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SHALLOW DISPOSAL OF RADIOACTIVE WASTE: SURVEY OF MODELS

by

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SHALLOW DISPOSAL OF RADIOACTIVE WASTE: SURVEY OF MODELS

ABSTRACT

A review and evaluation of computer codes capable of simulating the various processes that are instrumental in determining the dose rate to individuals resulting from the shallow disposal of radioactive waste was conducted. Possible pathways of contamination, as well as the mechanisms controlling radionuclide movement along these pathways have been identified. Potential transport pathways include the unsaturated and saturated ground water systems, surface water bodies, atmospheric transport and movement (and accumulation) in the food chain. Contributions to dose may occur as a result of ingestion of contaminated water and food, inhalation of contaminated air and immersion in contaminated air/water. Specific recommendations were developed regarding the selection and modification of a model to meet the needs associated with the prediction of dose rates to individuals as a consequence of shallow radioactive waste disposal. Specific technical requirements with regards to risk, sensitivity and uncertainty analyses have been addressed.

RÉSUMÉ

Le présent rapport fait état des résultats d'un examen et d'une évaluation des codes-machines capables de simuler les divers processus qui contribuent à déterminer le débit de dose que reçoivent des personnes à cause de l'évacuation peu profonde de déchets radioactifs. On a identifié les voies possibles de contamination, de même que les mécanismes qui contrôlent le mouvement des radionucléides dans ces voies. Les voies potentielles de transport comprennent les réseaux d'eaux souterraines non saturés et saturés, les masses d'eau de surface, le transport et le mouvement dans l'air (et l'accumulation) à l'intérieur de la chaîne alimentaire. La dose peut augmenter à la suite d'ingestion d'eau ou de nourriture contaminée, d'inhalation d'air contaminé et d'immersion dans de l'eau ou de l'air contaminé. Des recommandations particulières ont été mises au point au sujet du choix et de la modification d'un modèle. Des exigences techniques particulières ont également été abordées concernant les analyses de risque, de sensibilité et d'incertitudes.

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1. INTRODUCTION

The Atomic Energy Control Board (AECB) is a federal government agency responsible for regulating the use of nuclear power and the handling of radioactive material in Canada. As part of its mandate AECB is required to establish guidelines for, and eventually to license, radioactive waste disposal facilities. One method of evaluating the effectiveness of a particular site in controlling radionuclide releases and migration is through the use of numerical models. AECB has contracted with Geologic Testing Consultants, Ltd. (GTC) to evaluate and summarize available computer models that could be used to simulate the relevant physical and chemical processes which should be included in an evaluation of a shallow burial facility for radioactive wastes and to recommend a modeling strategy based on this review.

There are several pathways by which radionuclides could reach humans from radioactive wastes buried below land surface in shallow repositories (Figure 1). The ground-water pathway is certainly the most important potential means for radionuclide release to the surface environment, while radionuclide movement through the surface environment would predominantly occur through surface water (rivers, lakes, runoff etc.). Other mechanisms of radionuclide release and transport involve gaseous releases from decomposition of organic wastes, plant and animal intrusion, and erosion and transport by wind and surface water. Plant and animal intrusion may serve primarily to increase water infiltration rates and therefore somewhat enhance the ground-water pathway. Such intrusions, particularly by burrowing animals, can also result in radionuclides being brought to the surface where they may be dispersed by wind and water. Buried wastes could also potentially be uncovered by erosional processes. In any case, once radionuclides enter the surface environment, transport occurs primarily via surface water (including runoff) and atmospheric dispersion.

The purposes of this report are to review and evaluate the processes and existing models which represent all or part of the mechanisms described above and to recommend to the AECB an approach to a systems model which would represent all the important mechanisms of radionuclide movement and human exposure within a single software package, as well as provide the ability to perform uncertainty/risk analysis and various alternate calculations.

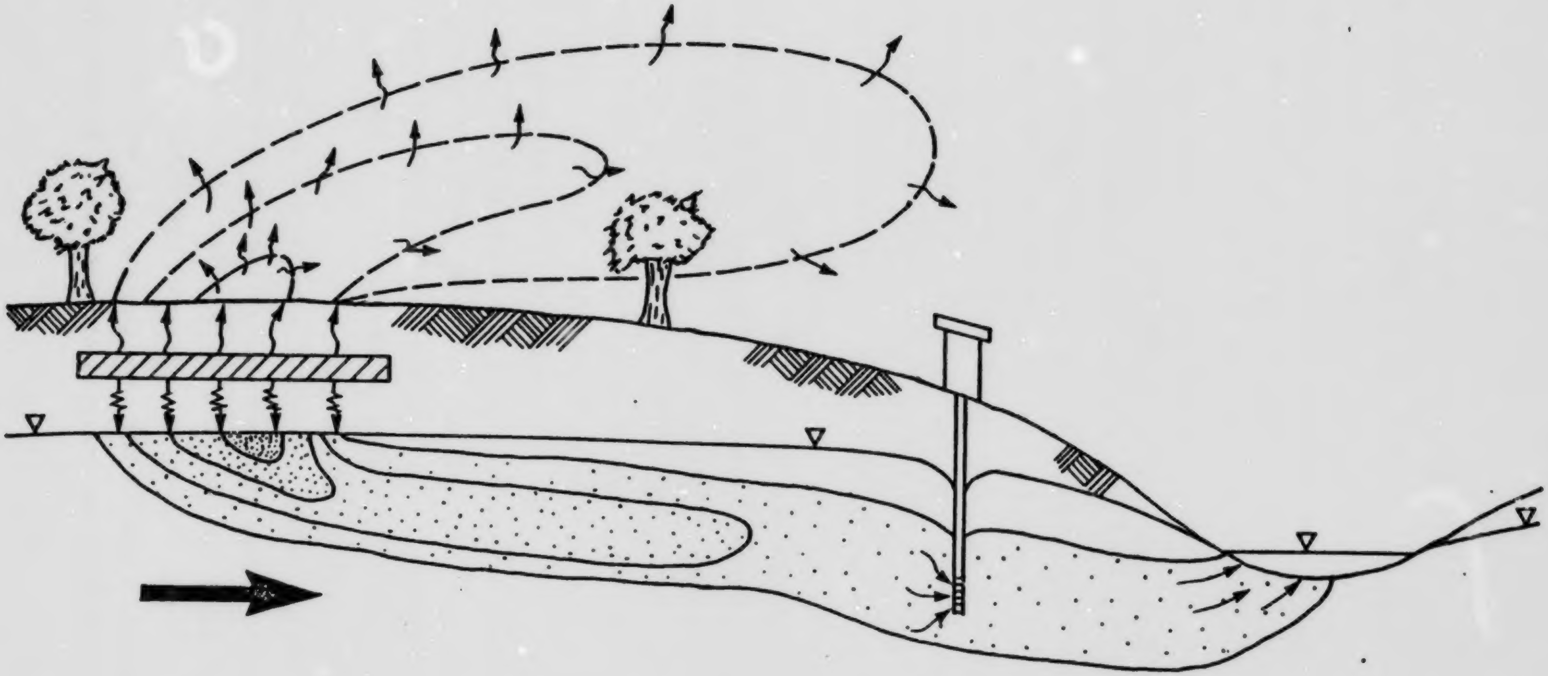


Figure 1. Illustration of Ground-Water and Atmospheric Dispersion Pathways

2. MECHANISMS OF RADIONUCLIDE RELEASE

Radionuclide release from radioactive waste disposal sites is possible through atmospheric transport, ground-water transport and surface water runoff. Atmospheric transport includes particulate as well as gaseous transport while surface water runoff considers dissolved radionuclides and suspended sediment transport. Ground water transport includes migration in the vapor and liquid phases in the unsaturated zone as well as dissolved radionuclide migration in the saturated zone. These transport processes, on an individual or sequential basis, will, in most instances, result in a potential exposure to man.

2.1 The Ground-Water Pathway

Radionuclide transport in shallow ground-water systems in Canadian terrain should generally consider the processes of advection, mechanical dispersion, molecular diffusion and geochemical retardation. The processes are operative and described at several scales in both the unsaturated and saturated ground-water regimes. The advective contaminant transport capacity of a ground-water system is usually described by the average linear ground-water velocity. Dispersion and diffusion of dissolved radionuclides both act as dilution mechanisms and are usually considered a single dispersion process in saturated, porous media flow. In unsaturated flow or in fractured media (such as tills and clays in the near surface) molecular diffusion (into, respectively, immobile waters and unfractured matrix adjacent to the fractures) is often considered as a process separate from mechaniccal dispersion. Mechanical dispersion (or mixing) results from the variations of water velocity which occur across and within an individual pore or fracture openings as well as due to the nature and extent of the interconnection and heterogeneities of the hydrogeologic media. Molecular diffusion, in response to concentration gradients, may be a relatively significant separate process in ground-water systems because the advective velocities are much lower than in surface water or in the atmosphere, and diffusion can significantly affect the distribution of radionuclides in a pore structure. Both mechanical dispersion and molecular diffusion typically result in a concentration reduction (or dilution) in the ground water system. Geochemical retardation in a hydrogeologic context is most often described by the distribution coefficient, which has a similar definition to the surface water distribution coefficient (see Section 2.3) and considers the same basic geochemical processes.

2.2 The Atmospheric Dispersion Pathway

Radionuclides may enter the atmosphere as a result of gaseous diffusion or as dust/windblown particles. Once in the atmosphere, the radionuclides will be subject to transport and mixing on a variety of scales. Much of the mixing or effective dispersion in the short to medium-range scales (less than 100 km) is due to turbulence or advective motions in the atmospheric boundary layer. The boundary layer (alternately the 'mixing' layer) is the layer within 0.5 to 2 km of the ground surface, characterized by a density stratification resulting from differences in temperature between the ground surface and the air. Under the simplifying assumptions of flat terrain, uniform wind velocity and complete 3-dimensional homogeneity the concentration distribution in any direction is Gaussian. However, complicating factors such as wind shear (velocity gradient), bouyancy (temperature gradient), mixing height, wind speed and other meteorological processes may need to be accounted for to adequately describe atmospheric transport. These factors are often accounted for by developing 'stability' categories, based on, for instance, vertical temperature gradients, and developing a relationship between the stability factors, the downwind distance and equivalent Fickian-type dispersion coefficients. Radionuclides can be removed from atmospheric transport through decay or deposition. Deposition occurs in three broad categories - sedimentation (for relatively large or dense particles), washout in association with rain or other forms of precipitation, and retention at the ground by processes such as impaction or adsorption.

2.3 The Surface Water Pathway

Radionuclide transport through surface waters such as streams, lakes or rivers considers the processes of radioactive decay, advection and dispersion of dissolved and suspended sediments, the movement of bed sediments, or 'bedload transport', as well as dissolved radionuclide interactions with the bottom sediments, suspended sediments and biomass. These processes can be conveniently subdivided into hydrodynamic and geochemical categories. From the hydrodynamic standpoint, the movement of any dissolved or suspended substance is related to the mean velocity of the water and the dispersion coefficient (or mixing length) which describes the variance about the mean of this typically normally distributed variable. In some instances the dispersion coefficient may also be considered a function of distance from a point or local source. The geochemical processes tend to describe (i) the reversible sorption capability of the sediment and bed material using a distribution coefficient concept which distributes the radionuclides between the liquid and solid phases, and (ii) the assimilative capability of the bed, or the non-reversible sorptive mechanisms. The geochemical mechanisms represented by the distribution coefficients or sink terms include ion-exchange, precipitation/dissolution, complexation/hydrolysis, oxidation/reduction, and colloid and polymer formation.

3. HUMAN EXPOSURE

3.1 Mechanisms

Human exposure via atmospheric pathways can include: (1) direct exposure from an overhead or ground-level radioactive plume, (2) inhalation of radionuclides, (3) consumption of foods (including meat and dairy products) produced from vegetation upon which radionuclides have deposited or vegetation grown in contaminated soil, and (4) direct exposure from radionuclides deposited on the ground. Human radiation exposure via the surface water pathway can include: (1) ingestion of contaminated water, (2) consumption of aquatic foods, (3) direct exposure by immersion in contaminated water, boating, or shoreline activities, and (4) ingestion of food contaminated by irrigation. Direct human exposure from the ground water pathway is primarily by ingestion of contaminated water, or ground water irrigated crops. Generally root crops do not penetrate to sufficient depths to make the uptake of contaminated ground water feasible. The ground water system however, provides a major pathway through which radionuclides may reach the surface water system.

3.2 Systems Model

To evaluate the radionuclide release mechanisms discussed above and estimate the potential effects on humans for tens or hundreds of years into the future requires the use of computer models to simulate the processes involved. The AECB is interested in a systems model that accounts for all of the important processes involved in evaluating radioactive waste disposal. This is to be accomplished in a single software package that is relatively easy and inexpensive to use. Figure 2 illustrates one possible suite of computer models and possible linkages that could provide the basis of such a systems model. Clearly other model couplings could be developed to perform the required analyses. For example, the source model and the direct-to-surface transport model may be combined in one computer program. Nevertheless, Figure 2 illustrates the important functions for a systems model and will be used for the following discussion of important model features and the use of such a systems model in sensitivity, uncertainty, and risk analysis. In the next section, the individual modules of a systems model as suggested by Figure 2 are briefly discussed. For each module, a description is provided of the important functions required of the module in order for it to fulfill adequately its role as part of a systems model. These descriptions are not intented to address all processes that might be simulated but rather to provide reasonable descriptions of minimal requirements for the individual modules.

3.2.1 Source Module

The purpose of the source module is to provide, as a function of time, the quantities and types of radionuclides available for transport in ground water or for direct transport to the surface. Therefore, this module must provide a time-dependent radionuclide inventory accounting for radioactive decay and production. To provide a source term for ground water transport (especially gas migration), the module must estimate the rate of gas production and the types and quantities of radioisotopes available to be carried to the surface in the gas.

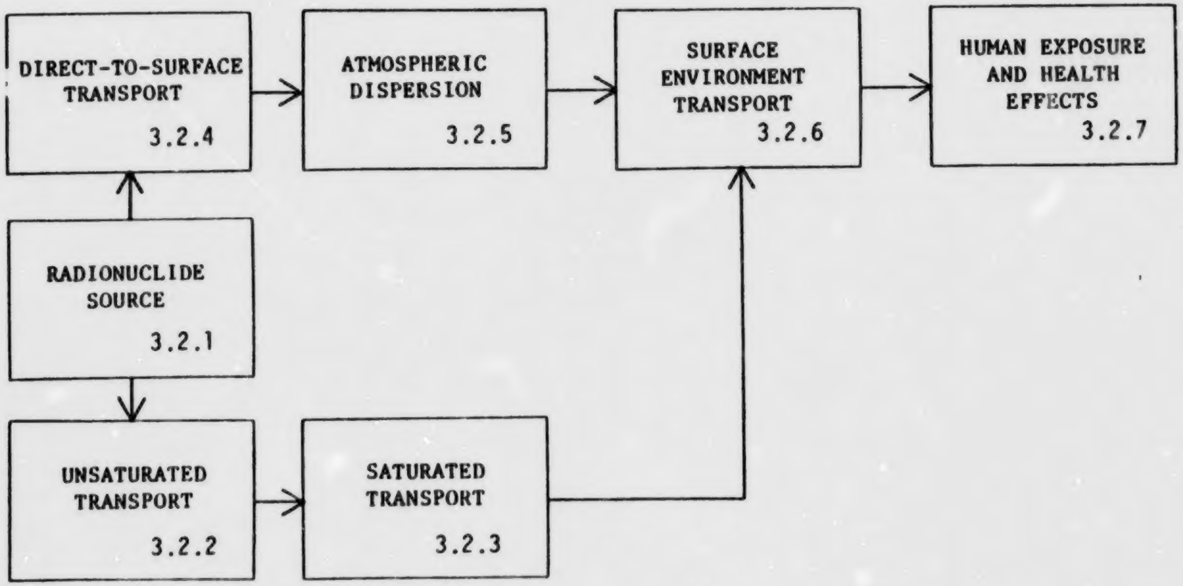

DIRECT-TO-SURFACE TRANSPORT
3.2.4
ATMOSPHERIC DISPERSION
3.2.5
SURFACE ENVIRONMENT TRANSPORT
3.2.6
HUMAN EXPOSURE AND HEALTH EFFECTS
3.2.7
RADIONUCLIDE SOURCE
3.2.1
UNSATURATED TRANSPORT
3.2.2
SATURATED TRANSPORT
3.2.3

Figure 2. A Possible Structure of a Systems Model

3.2.2 Unsaturated Transport Module

The purpose of this module is to simulate transport of radionuclides from the emplaced wastes (source) through the unsaturated zone to the water table. The module must take into account the water flow rate which is generally derived from the flow equation for unsaturated media. Radioactive decay and production should be treated along with radionuclide retardation through sorption on stationary soil grains. Retardation that can result from radionuclide diffusion into immobile water might also be treated.

3.2.3 Saturated Transport Module

The purpose of this module is to simulate radionuclide transport in the saturated zone to a discharge point to the surface environment. The module should treat both advective and dispersive transport, radioactive decay and production, and radionuclide retardation through sorption. The module should be able to represent discharge to the surface environment at surface water bodies (rivers or lakes) and at water wells.

3.2.4 Direct-to-Surface Transport Module

The purpose of this module is to represent radionuclide movement directly from the waste (source) to the surface. Such transport could occur by gaseous diffusion from the source or by direct exhumation (e.g., by erosion, burrowing animals, etc). Thus, the module relies on the time-dependent inventory of radionuclides remaining in the disposal site provided by the source module. The module might also estimate inventory fractions moved to the surface by various mechanisms.

3.2.5 Atmospheric Dispersion Module

The atmospheric dispersion module would simulate radionuclide transport in the atmosphere, provide time-dependent estimates of radionuclide concentrations in the contaminant plume, and estimate concentrations on the land surface that result from applicable deposition processes. The module should be able to account for both gaseous and suspended particulate sources. It should simulate dispersion accounting for wind speed and direction, and atmospheric condition.

3.2.6 Surface Transport Module

The purpose of this module is to define the modes of nuclide transport through the various surface pathways. Radionuclides may enter the surface environment via discharge of nuclide-carrying ground waters to rivers and lakes, withdrawal of radioactive well water, and deposition of particles carried through the atmosphere onto plants, soil and water bodies. Surface water is an important surface environment transport mode by which nuclides (either dissolved or adsorbed onto sediment) could be distributed throughout a region. Crop irrigation and livestock watering would provide transport pathways into biological receptors which are part of the human food chain. In addition to food chain pathways, direct ingestion of and immersion in radioactive water are other important surface pathways to man.

3.2.7 Health Effects - Dose-to-Man Module

The purpose of this module is to define human exposure parameters and the health effects that result from such exposure. Doses may be calculated as functions of nuclide concentration in food products and water, ingestion rates, and specific dose factors for nuclides. The nuclide concentrations in plants used for food are functions of application rates of radioactive water, deposition rates from atmospheric transport, the depositional history of the site and plant-specific uptake characteristics. Concentrations in meats, milk and eggs are functions of drinking water concentrations, concentrations in feed products and animal-specific uptake characteristics. Ingestion rates would be based on population averages to determine an average adult's and an average child's ingestion rate. Under most circumstances, these would be treated as constants.

Dose commitments to organs and to the entire body would be based in ICRP dose commitment models. These models were developed by the ICRP in 1959 (ICRP-2) but more recent ICRP literature (1979) suggests that some of these models may need review.

4. SYSTEMS MODELS: STATISTICAL CONSIDERATIONS

There are considerable uncertainties associated with many, if not most, of the input variables to the modules which make up a systems model for evaluating shallow radioactive waste disposal. Many of these input variables may be relatively unimportant in the sense that the model output is not very sensitive to them. However, important input variables to which the model is known to be sensitive (e.g., distribution coefficients and waste leach rates) may also be subject to considerable uncertainties. Therefore, risk estimates obtained from the systems model may be subject to large uncertainties. The use of point (or 'best estimate') values of important input variables has the effect of ignoring input uncertainties. When only 'best estimate' input results are used, the assumption is tacitly made that 'best estimate' output results are obtained. However, many realistic examples can be given to illustrate the fact that 'best estimate' input does not generally produce 'best estimate' output.

Consider the following simple example. Assume that a total mass (M_o) of a radioactive substance is instantaneously placed in solution in ground water. Such a simplistic assumption might approximate the leaching of toxic material from a shallow radioactive waste burial site during a rain storm. Assume further that, ignoring dispersion, a time interval T is required for a non-dispersed contaminant to migrate to a nearby stream. Suppose now that it is desired to estimate the total mass M of radioactive material discharging to the stream. Quantity M is estimated as

$$M = M_o e^{-\lambda TR}; \quad T = L/v$$

where λ is the radioactive decay constant, L the length of the migration path, v the average fluid velocity, and R the retardation factor. We now have an extremely simple assessment model where the performance measure is defined as the total mass of dissolved radionuclide which enters the stream. To examine the effects of input uncertainties on model output, assume the numerical values M_o = 1000 gm, λ = 0.001 yr^{-1} and T = 100 yr. As retardation factors are generally less well known, assume that values for R ranging from 10 to 100 are reported in the literature for the radionuclide of interest. Actually, the ranges of uncertainty for retardation factors (or equivalently, distribution coefficients) for real substances are often considerably larger than the range assumed here. The midpoint of the reported range of values for R (i.e., R = 55) could be used as a best estimate. Then based on the best estimate value of R, the total mass of radioactive contaminant discharged to the stream is calculated as M = 4.1 gm.

To examine the effects of the uncertainty in R on the estimated value of M, the simple assumption of a uniform distribution of values of R on the range from 10 to 100 was used. A total of 1000 calculations of M were performed using Monte Carlo (random) sampling of values of R from the uniform distribution. From these 1000 calculations the maximum calculated value of M was 367 gm. The minimum calculated value of M was 0.0454 gm and the mean of the 1000 output values was 40.2 gm. Note there is almost a factor of 10 difference between the calculated value of M based on best estimate input and the sample estimate of the mean value of M with uncertainties in input values.

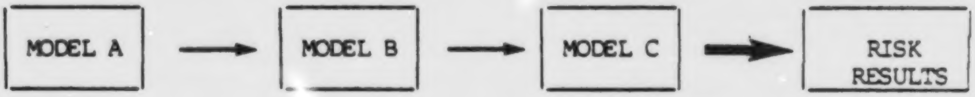
The above discussion simply illustrates the fact that 'best estimate' inputs to a systems model may not adequately represent the system, but rather that the system may be much more adequately represented in its entirety (and uncertainty) by utilizing all the information available, i.e., by statistically representing the parameters and input conditions.

Any systems model used by AECB must be structured in such a way that input data uncertainties can be taken into account in a relatively convenient manner. There are several techniques available for addressing sensitivity and uncertainty analysis. Differential techniques that provide partial derivatives of model output with respect to input variables can be highly valuable for examining model sensitivity (INTERA, 1983) when large numbers of input variables are involved and model output is not a highly nonlinear function of model input. In such applications, the calculated partial derivatives can also be used (by first order Taylor expansion) to estimate model output variation that would result from relatively small variations of model input parameters. However, the output from shallow radioactive waste disposal systems models can be expected to be a highly nonlinear function of input because of the interaction of variables such as leach rates, dispersion parameters, and distribution coefficients combined with the exponential variation of radionuclide concentrations due to radioactive decay.

Furthermore, uncertainties on input variables may be quite large. For these reasons, differential techniques would be of very limited use for estimating output uncertainty.

An alternative approach, more directly suited to uncertainty analysis than differential methods, is represented by stochastic modeling (Dettinger and Wilson, 1981). In such models, the governing differential equations are written in terms of the mean and variance of input and output. Thus, by using means and variances (and perhaps correlation) of input variables, such models provide means and variances of output quantities. The major drawback to such models is the difficulty and expense involved in their development. Furthermore, stochastic models are generally complex and require considerable computer memory and run time.

For the reasons cited above, a more tractable approach to uncertainty and risk analysis involves the use of statistical sampling methods. One such sampling approach is briefly described here as an example to illustrate some of the important concepts involved. The series of models (or modules involved in the system model calculations) are represented below as unspecified Models A, B and C.



Model A could be a combination source and ground-water transport model, model B could be a surface-water transport model and Model C could be used to calculate human exposure and health effects.

The first step in this systems uncertainty analysis example would be to list the important variables for Models A, B and C. These are the variables which will be treated as random variables in the uncertainty analysis. Figure 3 illustrates such a variable list where variables X_1 through X_i are associated with Model A, X_{i+1} through X_j are associated with Model B and X_{j+1} through X_k are associated with Model C. Also illustrated in Figure 3, is the fact that distributions representing the uncertainties in these variables must

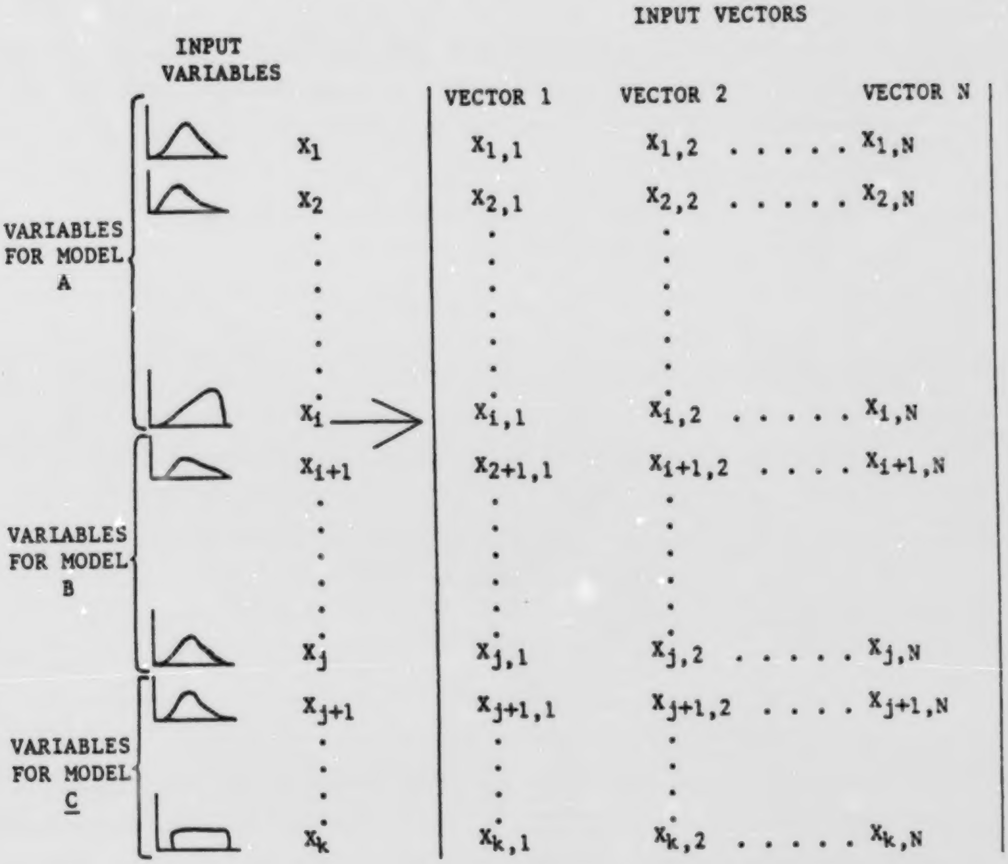

INPUT VECTORS
INPUT VARIABLES
VECTOR 1
VECTOR 2
VECTOR N
VARIABLES FOR MODEL A
VARIABLES FOR MODEL B
VARIABLES FOR MODEL C
x_1
$x_{1,1}$
$x_{1,2}$ . . . . . $x_{1,N}$
x_2
$x_{2,1}$
$x_{2,2}$ . . . . . $x_{2,N}$
x_i
$x_{i,1}$
$x_{i,2}$ . . . . . $x_{i,N}$
x_{i+1}
$x_{2+1,1}$
$x_{i+1,2}$ . . . . $x_{i+1,N}$
x_j
$x_{j,1}$
$x_{j,2}$ . . . . . $x_{j,N}$
x_{j+1}
$x_{j+1,1}$
$x_{j+1,2}$ . . . . $x_{j+1,N}$
x_k
$x_{k,1}$
$x_{k,2}$ . . . . . $x_{k,N}$

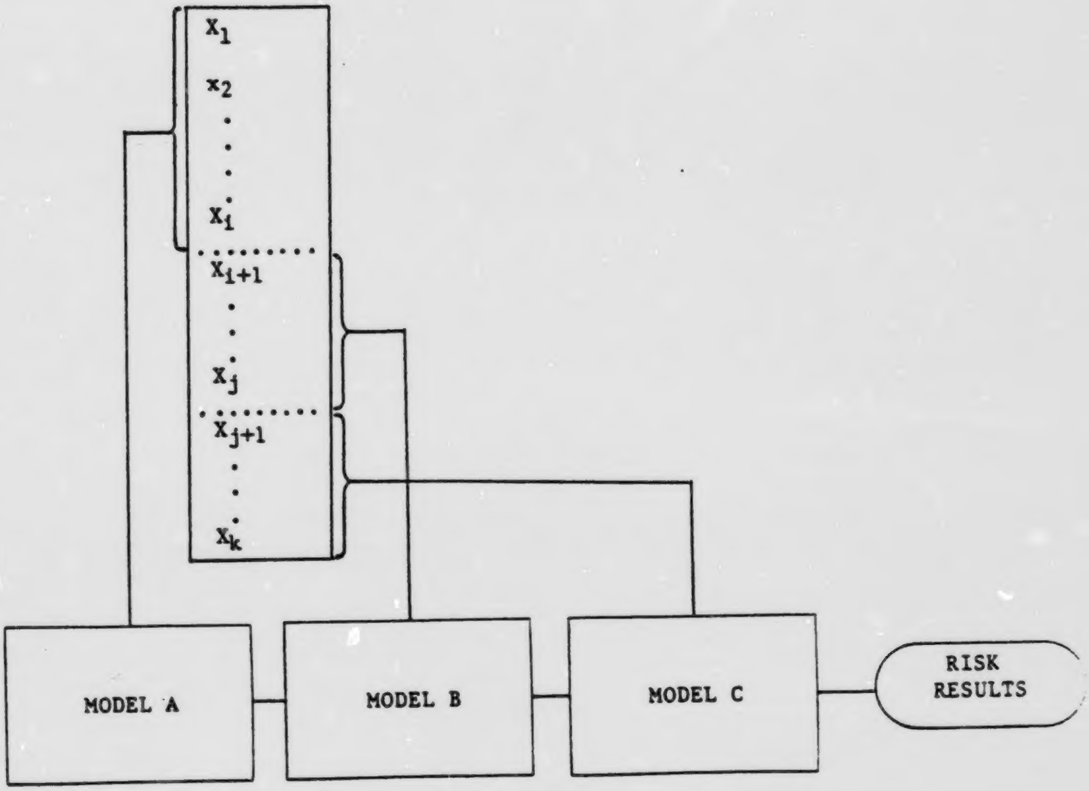
Figure 3. Example of Input Variable Sampling

be assigned to provide a basis for sampling input values. In performing actual risk/uncertainty analysis, these input variable distributions would be developed from available data or, where such data are lacking, best engineering judgment.

Given input variable distributions to be sampled, we assume that a total of N computer runs are to be made. In practice, the number of runs required will be based on the number of variables to be sampled, the sampling method used, and anticipated computer costs. Figure 3 illustrates the formation of N input vectors. An input vector may be defined as an array consisting of k numerical values, one for each of the k input variables, sampled from the input variable distributions. An input vector could be formed by randomly sampling a value of X_1 from its distribution, then randomly sampling a value of X_2 from its distribution and so on. When a value has been sampled for each of the k input variables (X_1 to X_k), one input vector has been formed. Once N input vectors have been formed, N complete calculations involving the entire sequence of models can be performed. The use of input vectors in these calculations is shown in Figure 4 which illustrates a single run of the model sequence. For a particular input vector, the values for X_1 through X_i are used (along with other data as appropriate) as input to Model A. The results of Model A along with values for X_{i+1} through X_j provide input to Model B. The output from Model B together with values for X_{j+1} through X_k provide input to Model C. Thus, the sequence of three models is treated as a single systems model and one systems model run is made for each input vector.

The example above assumed simple random or Monte Carlo sampling of the input variables. While Monte Carlo sampling is relatively inefficient compared to some other sampling schemes, it has the advantages of being simple and easy to present. Newer techniques such as Latin Hypercube Sampling (LHS) can also be used (McKay, Conover and Beckman, 1979). The concept of Latin Hypercube Sampling can be illustrated by the following example (Figure 5).

Consider a simple two variable case and assume that 4 input vectors will be generated. For the present example, an input vector is simply a pair of numerical values; one value selected from the range of variable X_1 and one value selected from the range of X_2. To perform the Latin Hypercube Sample, the range of each variable is first divided into four non-overlapping intervals based on equal probability as shown in the following illustration.



X_1
x_2
X_i
X_{i+1}
X_j
X_{j+1}
X_k
MODEL A
MODEL B
MODEL C
RISK RESULTS

Figure 4. Illustration of the Use of an Input Vector in a Systems Model

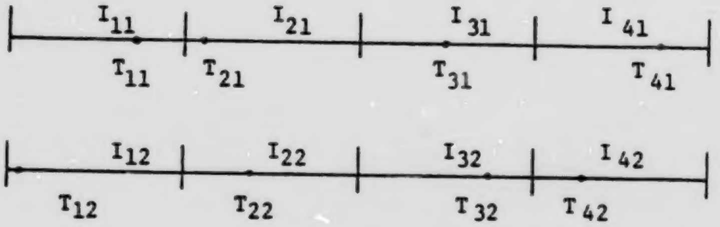

I_{11}
I_{21}
I_{31}
I_{41}
T_{11}
T_{21}
T_{31}
T_{41}
I_{12}
I_{22}
I_{32}
I_{42}
T_{12}
T_{22}
T_{32}
T_{42}

Figure 5. Illustration of Latin Hypercube Sampling for Two Variables

Values T_{ij} are randomly selected according to the distribution across the interval from intervals I_{ij} as shown above. Finally, 4 input vectors (T_{k1}, T_{m2})k,m = 1,2,3,4 are formed by randomly selecting, without replacement, from the 4 previously selected values of X_1 and X_2.

The choice of LHS or Monte Carlo techniques rests largely with the type of application. For sampling input variable distributions of known sample size, LHS should be used. The reason for this is that, given the same sample size, LHS produces estimates with smaller mean square error than does Monte Carlo. Thus, desired representations of input and output variable distributions can be obtained using LHS with smaller sample sizes than required by Monte Carlo sampling.

If the cost of computer usage becomes a concern, an efficient sampling technique such as LHS can therefore provide the necessary risk/uncertainty analysis results with considerably fewer computer calculations. Monte Carlo sampling is most useful for applications for which the sample size is not known a priori. An example is a decision tree in which the decision at a node depends upon a value sampled from some distribution. The number of times the sampling must occur (sample size) may depend on decisions made at previous nodes.

Although LHS is recommended for generating input vectors, ideally Monte Carlo sampling should also be available to the systems model. There are two reasons for this. First LHS is still a relatively new technique and is not particularly widely known. If questions should arise concerning its use, Monte Carlo sampling is widely understood and should, therefore, be readily available as an option. The second reason is based on the fact that an LHS sample of size one is equivalent to a single Monte Carlo sample. Thus, LHS sampling software can be easily adapted to also provide a Monte Carlo sampling capability.

The above discussions concerning statistical sampling have focused on uncertainty and risk analysis. In either case, the primary statistical objective is the creation of a systems model output distribution function. There are other statistical considerations that should significantly influence the development of the systems model, namely, sensitivity analysis and correlations among input variables. The importance of sensitivity analysis stems from the fact that not all input variables will have a strong influence on output variation. Therefore, before trying to characterize uncertainties in all input variables, it is essential that important input variables be identified. This is best achieved by performing sensitivity analysis using the system model. By 'sensitivity analysis', we mean the study of variation in model output with respect to model input (Inman, Helton and Campbell 1981). Sensitivity analysis must also take into account the level of uncertainty in the input variables. Thus, even though model output may be sensitive to a particular input variable, if the variable is well defined it may have little effect on model output uncertainty. Thus, within the context of sensitivity analysis, an 'important' input variable is one which, when allowed to vary over its allotted range of uncertainty, has significant influence on model output variation.

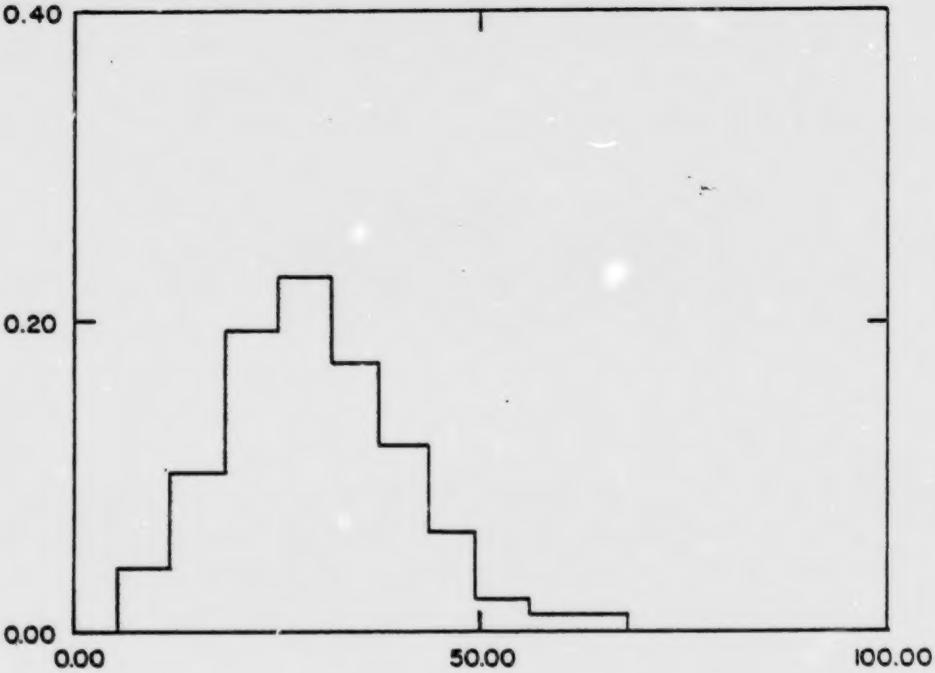
One technique that has proven valuable in assessing input variable importance is the use of partial rank correlation coefficients. The partial correlation coefficient provides a measure between -1 and 1 of the extent to which a particular input variable can form a linear approximation to the output variable. The simple correlation coefficient provides a similar measure. However, in calculating the simple correlation, the fact that several input variables are allowed to change simultaneously is ignored. Therefore, the influence of a particular input variable on model output, as measured by the simple correlation coefficient, may be masked by the simultaneous variation of other input variables. Partial correlation coefficients, on the other hand, systematically eliminate the effects of varying input variables other than the variable in question. However, while partial correlation coefficients provide a relative easy means to examine linear relationships between model input and model output, they can be misleading for nonlinear relationships. For the component modules of the systems model, model output is expected to be monotonic but not necessarily linear with each of the input variables. For this reason, a procedure that reveals monotonic rather than linear relationships is needed. Such a procedure is provided by calculating partial correlations on ranked data (Iman and Conover, 1979). The concept of the rank transformation is simple in that values of each variable (input and output) are replaced by their corresponding ranks. For example, the smallest value of input variable X_1 is replaced by rank 1, the next smallest by rank 2, and so on. In the case of ties, average values are assigned. The effect of the rank transformation is to linearize the relationship between the output variable and an input variable when that relationship is monotonic. Monotonicity is now an expected property of the systems model. Thus, if variable values are replaced by their ranks, partial correlations on these ranks can provide a meaningful measure of sensitivity of model output to model input.

The system model should offer the option of calculating partial rank correlation coefficients at the output of each module. Thus, referring to the example represented in Figure 4, the user should be able, using partial rank correlations, to examine sensitivity of Model A to its input (X_1, X_2, ..., X_i), or the sensitivity of Model B output to its input (X_{i+1}, X_{i+2}, ..., X_j) and any of the input to Model A, or the sensitivity of the final risk results to any of the systems model input variables. This capability will simplify uncertainty and risk analysis by helping eliminate unimportant variables from consideration. Furthermore, this sensitivity analysis capability will help identify areas where better data are needed to reduce output uncertainty.

As a final statistical requirement, there should be a capability to account for correlations among input variables. In particular, use of rank correlations is recommended (Iman and Conover, 1980) for reasons cited above. Furthermore, variable correlations are often imposed as a result of expert opinion and intuition rather than from observed data. Opinion and intuition usually follow the example form: for a significant positive correlation, when variable 1 is at the upper (lower) end of its range, variable 2 ought to be at the upper (lower) end of its range most of the time. Correlating the ranks of variables 1 & 2 has this effect.

The impact of imposing or neglecting correlations is demonstrated in Figure 6. The model used was a simple multiplication, $Z = X \cdot Y$. Figures 6a, 6b, and 6c show the histograms for the response variable Z that result from imposing correlations on X and Y of size 0.0, 0.75, and -0.75, respectively. The effect on the variation in the variable Z is evident from the graphs (in spread and height) and in the estimated standard deviation.

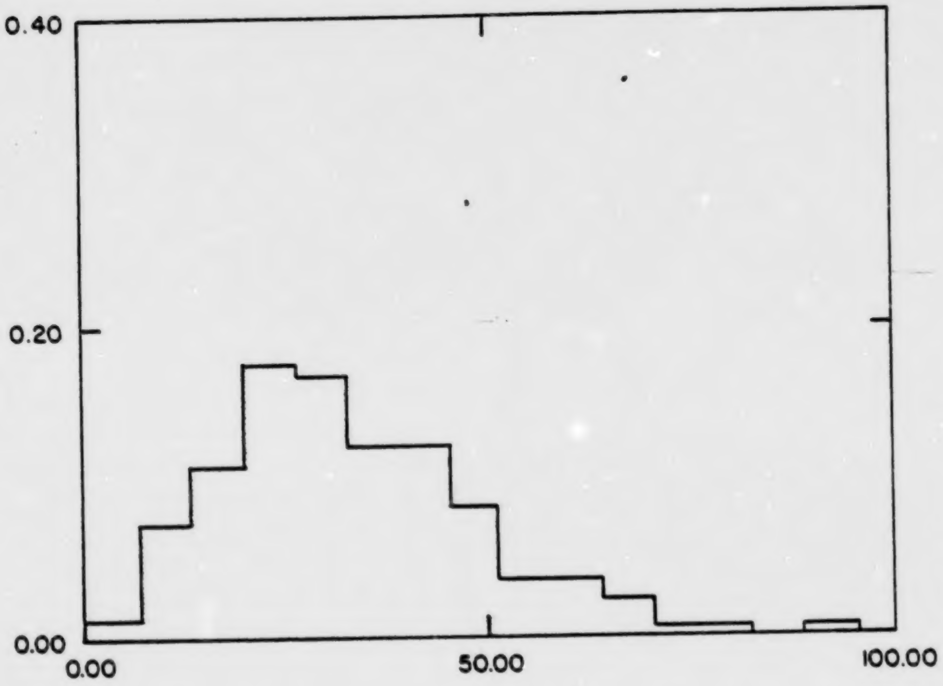
This simple example points out the importance of correlations. Neglecting correlations may over- or under-estimate the uncertainty of output. In Figure 6b high (low) values of X were generally paired with high (low) values of Y yielding a greater quantity of large (small) values for Z and, hence, spreading Z over a larger range. The opposite effect is evident in Figure 6c.



RESULTS FROM 200 TRIALS

MINIMUM	MAXIMUM	MEAN	STD. DEV.
6.95344	65.8762	30.27346	11.49829

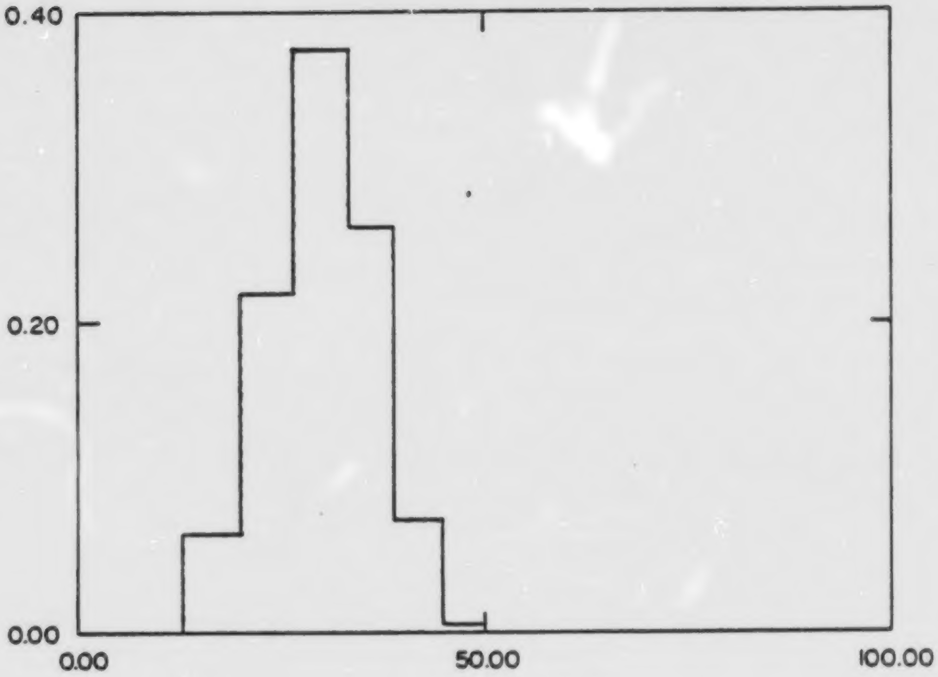
Figure 6a. 0.0 Correlation



RESULTS FROM 200 TRIALS

MINIMUM	MAXIMUM	MEAN	STD. DEV.
4.151512	70.90401	31.83356	15.23282

Figure 6b. 0.75 Correlation



RESULTS FROM 200 TRIALS

MINIMUM	MAXIMUM	MEAN	STD. DEV.
14.01173	48.32173	28.70125	6.171938

Figure 6c. -0.75 Correlation

This discussion on statistical considerations has been developed for the purpose of providing background on which to evaluate existing individual module model capabilities, as well as the overall system model capabilities in the next section. Although, many of the models evaluated are not currently statistically oriented, the relative ease with which these could be adapted for statistical studies has been factored into the recommendations.

5. AVAILABLE MODELS

The models evaluated as part of this survey were selected based on the following general criteria:

1. Processes Considered - the model must consider at least one of the processes (i.e., source term, ground water flow and transport, surface water transport, dose-to-man) and the major mechanisms of the process, identified as being pertinent to shallow waste storage facilities;
2. Documentation - adequate documentation is available to describe the numerical implementation of the code, the assumptions and limitations of the code, and a comprehensive user input guide;
3. Flexibility - the model should be flexible in terms of its geometry, boundary conditions etc., so as to be applicable to most sites likely to be encountered in Canadian terrain.
4. Non-proprietary - the model should be available for use by the general public.

While these criteria were generally used to screen models for inclusion in the evaluation they were not meant as absolute guidelines, and in some cases models which violate the criteria were also included due to other compensating factors, for example, outstanding technical merit. Where this has occurred the reason for selection has been noted in the model survey. Model summaries (Appendix A) were constructed for each model that was reviewed and did not violate the above criteria. The model summaries are generally brief although some are more detailed than others. The level of detail provided for each model is very much a function of the available documentation and potential applicability of the code. The more detailed summaries include a list of input/output variables, a description of the code, existence of a quality assurance (QA) system, programming language and system, sponsoring agency, available validation and verification studies, author/contact and address, review reference and documentation. The brief summaries consist of a short description of the code, author/contact and address, the review reference and documentation reference. Only when model verification or validation was reported (in the review reference) was this information included in the brief model summaries. If no reference is made to model verification or validation it indicates that no such information was reported in the review reference. Generally, more detailed model summaries were compiled for models such as systems models. The capabilities of the various module models are summarized in Appendix A, Tables 1 through 6 while the systems models' capabilities are summarized in Table 7.

The model survey was undertaken using, as much as possible, the results of previous model surveys conducted to examine models applicable to radioactive waste repositories, ground-water transport, atmospheric transport, surface water transport and dose-to-man calculations. The rationale for this approach was to efficiently identify models that could potentially meet AECB's needs. The model summaries are based on the information presented in all of the reviews.

The models included in this compilation are typically models that have been developed and are used by various governmental agencies and national laboratories. Such codes are readily available to the public and are usually well documented, and tend to gain wider acceptance throughout the scientific community. Models developed at various academic institutions, while they may be technically very sound, typically are not well documented and not widely used. (These are observations of what was found during the model survey and were not used as objectives in selecting models.)

Finally, it should be stressed that the model survey is not by any means exhaustive, nor is it intended to be. The survey is meant to identify models that represent the state-of-the-art with regard to radionuclide migration from a shallow land burial facility. Consequently, the survey contains descriptions of several, but not necessarily all, models representing each of the possible model types for a specific process. Due to time and budget limitations, the discussion of individual models' capabilities remain in Appendix A, Tables 1 to 7. A brief discussion of the system models evaluated in Appendix A, Table 7 is presented below.

A total of eight systems models were examined. The models are; AMRAW, CALMAC, HERMES, NRC-LPGS, NRC-Sandia Risk Assessment Methodology, NUTRAN, PRESTO and SYVAC. All of these systems models appear to fall short to some extent of the AECB's needs. Several (AMRAW, NUTRAN, SYVAC, and the SANDIA-NRC systems model) were developed for deep geologic disposal of high-level waste and therefore do not consider the atmospheric dispersion pathway. SYVAC is currently being modified by AECL's Applied Mathematics branch at Chalk River Nuclear Laboratories for application to shallow land burial facilities. However, at this time, this work is incomplete and the exact nature of the changes have not been finalized. CALMAC does not consider decay chains (i.e., does consider radioactive decay but not generation of daughter products) and is designed to calculate the radioactive waste concentration in a disposal site to assure dose limits are not exceeded. HERMES addresses problems associated with nuclear facility siting. Thus, the treatment of the source and the ground-water pathway in HERMES may be inadequate for AECB's needs. The NRC-LPGS model considers liquid pathways and is designed for analysis of potential reactor accidents. PRESTO appears to be the only systems model examined that was specifically developed for shallow burial of radioactive wastes. However, PRESTO does not consider generation of radioactive daughter products in long-lived decay chains.

Despite the fact that all the systems models suffer from some shortcomings, there are several that have strengths worthy of consideration. NUTRAN has some built-in capability for treating scenarios (i.e., events that alter the state of the physical system and thereby affect radionuclide release). SYVAC has been designed to consider input variable uncertainties by performing Monte Carlo sampling to generate an output distribution. The SANDIA-NRC systems model is designed to use Latin Hypercube Sampling (LHS) or Monte Carlo sampling of input variable distributions, allows correlation among input variables, and evaluates sensitivity of output to input while generating the output distribution function. The NWFT/DVM source and ground-water transport model has considerable capabilities while still remaining efficient for use in risk analysis.

6. RECOMMENDATIONS

6.1 General Recommendations on Systems Models

Before moving to specific recommendations, it is useful to first make some broad recommendations concerning an appropriate systems model for analyzing shallow disposal of radioactive wastes. The first point is that the systems model should be structured in a modular format. That is, the major systems model components (e.g., ground-water transport, atmospheric dispersion, etc.) should be incorporated as distinct modules. This requirement should be met regardless of whether the system model is a single computer program or several programs that interface via input/output files. If the systems model is a single program, the major computational modules should occur as distinct subroutines or groups of subroutines. A modular structure will assure that as improved computational capabilities become available outdated modules can be easily replaced without requiring a major systems model rewrite.

The second point involves the intended use of the systems model in uncertainty and risk analysis. Because the procedures discussed in Section 4 and recommended in Section 6.2.1 involve the use of statistical sampling, applications of the systems model will generally involve multiple runs. This type of use implies that the systems model must be efficient in both computer time and in user time required to set up and execute a problem. Therefore, the individual computational modules or submodels of the systems model must be relatively simple in terms of required input data and must require little computer time per calculation. This recommendation embodies one of the most difficult aspects of developing a systems model; namely, acquiring submodels that are sufficiently realistic to assure that the systems model results are realistic while being simple enough to be practical for use in a systems model context.

The requirements of simplicity and efficiency for components of a systems model lead to a third important general recommendation. To assure technical credibility for systems model results, it may be necessary to have more sophisticated and comprehensive models available for back-up analyses. For example, a two- or three-dimensional ground-water flow model may be needed to establish flow directions and fluid velocities in order to assure meaningful results from a simplified radionuclide transport model. Or a source model, suitable for use in a systems model, may have relatively simple source rate options such as constant rate, exponential leach rate, or user-supplied source rate. However, a more sophisticated source module might be used to develop time-dependent source rates for use in the simpler source module of the systems model.

6.2 Specific Recommendations

6.2.1 Statistical Methods

The most tractable approach for uncertainty and risk analysis is to employ statistical sampling methods. This essentially means that the systems model would consist of a series of deterministic models which represent the important processes in a sequential fashion with output from one model providing input to the next in the series. The last model in the series calculates health effects. To produce an output distribution function for health effects (i.e., risk results), multiple systems model runs are performed. The input for those runs is obtained by statistically sampling user-supplied distributions for systems model input parameters. Both Monte Carlo and Latin Hypercube sampling methods should be available as options for generating input vectors for the systems model.

For "sensitivity analysis", or the study of variation in model output with respect to model input, the relative importance of input variables can be assessed through the use of partial rank correlation coefficients. The systems model should offer the option of calculating partial rank correlation coefficients at the output of each module, as well as the ability to use rank correlations with the input variables.

6.2.2 Existing Systems Models

The most promising systems model appears to be PRESTO which has several important advantages. First, it is designed explicitly for shallow burial of radioactive wastes. Thus, scenarios unique to this waste disposal problem can probably be more realistically addressed with PRESTO than any of the other systems models examined here. The fact that the current version of PRESTO treats only normal operation (versus breachment scenarios) with operational spillage could lead to difficulties in adapting a current version of the model to consider intrusion scenarios. Later versions will also consider site reclamation by farming, human intrusion, and erosion followed by atmospheric suspension. However, the scenario currently modeled is probably the most important. Another advantage of the PRESTO model is the fact that it is being developed at the Oak Ridge National Laboratory (ORNL). ORNL has considerable experience in evaluating shallow burial of radioactive wastes. Furthermore, ORNL has long been a technical leader in simulating atmospheric and surface water transport of radionuclides and in calculating human exposure and health effects.

Two potential weaknesses of PRESTO, namely, its ground-water transport capability and suitability for risk, sensitivity and uncertainty analysis can be remedied. The ground-water transport capability could be strengthened by replacing its current treatment with either NWFT/DVM or UCB-NE-10/UCB-NE-30. Both have the capability to treat decay chains and a variety of source terms. NWFT/DVM has the added advantages of considerable use and verification and the potential for simulating both unsaturated and saturated transport. Adaptation of PRESTO for risk, sensitivity and uncertainty analysis would depend first on the model's computational efficiency. Assuming adequate efficiency (i.e., cost per simulation is not prohibitive), it should be straightforward to add a capability for Latin Hypercube and Monte Carlo sampling along with the other statistical capabilities recommended in Section 6.2.1.

PRESTO would be best suited to analyze shallow burial facilities. This is evidenced by its treatment of the unsaturated zone and its simplified saturated ground water models. If sufficient changes were made it is conceivable that the model could be applied to intermediate depth disposal facilities.

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Appendix A

Model Summaries

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GTC

NUCLIDE INVENTORY

MODEL SUMMARIES

CHAINS

Model Type: Nuclide Inventory

Author:
W.B. Henderson
Nuclear Analysis
Westinghouse PWR Systems Division
P. O. Box 355
Pittsburgh, PA 15230

Sponsoring Agency: Unknown

Description: This model calculates the existing nuclide inventory as a function of time by solving the Bateman equations analytically. The model is limited to 50 members in a chain, 100 energy groups and 100 time values.

Review Reference: SAI

Documentation: Henderson, W. B., 1967. Program CHAINS, (NMP-856), GEMP-490, March 27.

CINDER

Model Type: Nuclide Inventory

Author:
T.R. England
Los Alamos Scientific Laboratory
P. O. Box 1662
Los Alamos, NM 87545

Sponsoring Agency: EPRI, USDOE

Description: This model calculates fission products, actinide inventories and depletion.

CINDER is the LASL nuclide depletion code and is used to predict nuclide buildup and decay in and out of neutron flux. The code predicts nuclide curies, beta, gamma, and alpha heating and spectra, and neutron absorption. The code treats cross sections in four or more groups and decay energies in multigroups. Flux and cross sections can be time-dependent. Branching can be by absorption or decay. CINDER is very general in its ability to duplicate specified power flux histories for any set of coupled nuclides. Nuclides not in the library must be specified in detail, including parameters and the type of coupling.

Review Reference: SAI

Documentation: Reports: EPRI NP-356, Electric Power Research Institute, Palo Alto, CA, and LA-6745-MS and LA-6746-MS, Los Alamos Scientific Laboratory, Los Alamos, NM.

ISOGEN

Model Type: Nuclide Inventory

Author: H.H. Van Tuyl
Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: This model calculates radioisotope generation and decay using two group neutron cross-sections. The model uses modified Bateman equations along with a chain-tracing technique allowing feedback and branching at any nuclide. The model is limited to 30 times steps for irradiation and decay, 50 member chains or a maximum of 500 nuclides per simulation. Accuracy is reported to be within 0.1 percent for any transmutation chain involving decay and/or neutron reactions.

Review Reference: CEC, SAI

Documentation: Van Tuyl, H. H., 1964. ISOGEN - A Computer Code for Radioisotope Generation Calculations, HW-83785, General Electric Company, Richland, WA.

ORIGEN2

Model Type: Nuclide Inventory

Author:
A.G. Croff
Oak Ridge National Laboratories
P.O. Box P
Building K-1001
Oak Ridge, TN 37830

Sponsoring Agency: ERDA

Description: This model calculates the radionuclide composition of a nuclear material during irradiation or decay. Other calculated variables include isotopic composition (by element), radioactivity, thermal power, neutron adsorption and fission rates, neutron emission from spontaneous fission and photon emissions in 18 energy groups. A matrix exponential technique is used to compute nuclide concentrations for long-lived isotopes. For short-lived isotopes the Bateman equations and secular equilibrium is used together with the assumption of constant cross-section. Nuclide libraries supplied with the code provide space and spectrum averaged cross-sections. One group-flux is assumed. This program has been distributed world wide and has been in use since the early 1970's.

Review Reference: CEC, SAI

Documentation:

Bell, M. J., 1973. ORIGEN -- The ORNL Isotope Generation and Depletion Code, ORNL-4628, Oak Ridge National Laboratory, Oak Ridge, TN.

Croff, A. G., M. A. Bjerke, G. W. Morrison, and L. M. Petrie, 1978. Revised Uranium-Plutonium Cycle PWR and BWR Models for the ORIGEN Computer Code, ORNL/TM-6051, Oak Ridge National Laboratory, Oak Ridge, TN.

Croff, A. G., R. L. Haese, and N. B. Gove, 1979. Updated Decay and Photon Libraries for the ORIGEN Code, ORNL/TM-6055, Oak Ridge National Laboratory, Oak Ridge, TN.

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ORIGEN2

Croff, A. G., 1980a. A User's Manual for the ORIGEN2 Computer Code, ORNL/TM-7175, Oak Ridge National Laboratory, Oak Ridge, TN.

Croff, A. G., 1980b. ORIGEN2 -- A revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code, ORNL-5621, Oak Ridge National Laboratory, Oak Ridge, TN.

Croff, A. G., et al, 1980. Alternative Fuel Cycle PWR Models for the ORIGEN Computer Code, ORNL/TM-7005, Oak Ridge National Laboratory, Oak Ridge, TN.

LEACHING MODEL SUMMARIES

BARIER

Model Type: Leach Model

Author: D.H. Lester
Science Applications Inc.
La Jolla, CA 91038

Sponsoring Agency: USDOE

Description: This model simulates the processes of material corrosion, temperature and stress on individual portions of high level waste packages. An estimate of the failure time of each barrier is calculated and when all barriers have failed the code simulates the release of nuclides from the damaged package. Leaching of waste material from damaged canisters is included. Transport through barriers is based on the analytic solution of a 1-D diffusion equation for slab geometry. Adsorption in the backfill is treated using retention factors.

Review Reference: CEC, SAI

Documentation: Stula, R. T., T. E. Albert, B. E. Kirstein, D. H. Lester, 1980. BARIER Code User Manual. Energy Systems Group, Science Applications, Inc.

Lester, D. H., R. T. Stula, and B.E. Kirstein, 1981. Supplement to BARIER Code User Manual.

American Society of Mechanical Engineers, 1977. ASME Boiler and Pressure Vessel Code, Section VIII, Div. 1.

QTERM

Model Type:	Leach Model
Author:	W. Lutze Hahn-Meitner-Institut fur Kernforschung Berlin Glienicker Strasse 100, D 1000 Berlin 39 West Germany
Sponsoring Agency:	Unknown
Description:	QTERM calculates a leach rate of a cylindrical block immersed in brine according to an empirically-derived equation. The program includes the effect of temperature and the resulting decrease in block radius.
Review Reference:	CEC
Documentation:	Altenhein, F. K., W. Lutze and R. C. Ewing. Long-Term Radioactivity Release from Solidified High-Level Waste - Part I. An Approach to Evaluating Experimental Data, in: Scientific Basis for Nuclear Waste Management V, Vol. II, W. Lutze ed., North-Holland Publ. Comp., New York 1982. Altenhein, F. K., W. Lutze and R. C. Ewing. Long-Term Radioactivity Release from Solidified High-Level Waste - Part II. Parametric Study of Waste Form Properties, Temperature and Time, in: Scientific Basis for Nuclear Waste Management VI, Vol. VI, D. G. Brookmis ed., North Holland Publ. Comp., New York, in press. Altenhein, F. K., W. Lutze and R. C. Ewing. Long-Term Radioactivity Release from Solidified High-Level Waste - Part III. The effect of Canister Lifetime. Submitted for Pub. to the American Ceramic Society, 85th Annual Meeting, Chicago, April 24-27, 1983.

SWIFT

Model Type: Ground Water Flow and Transport/Leach

Author: INTERA Environmental Consultants
11999 Katy Freeway, Suite 610
Houston, Texas 77079

Sponsoring Agency: USNRC

Description: SWIFT is three-dimensional model describing the transport of radionuclide chains through the groundwater (see model summary of ground water transport models for more complete description of this aspect of the model). The leach submodel of SWIFT assumes a constant fractional leach over a user-specified leach time and also considers solubility controls.

Review Reference: INTERA Environmental Consultants Inc, 1982. User Manaual for SWIFT, VERSION TUB/PTC, Release 3.82.

Documentation: As above.

GTC

WAPPA

Model Type:	Leach Model
Author:	Arthur D. Little, Inc. Acorn Park Cambridge, Massachusetts 02140
Sponsoring Agency:	USDOE
Description:	The WAPPA (Waste Package Performance Assessment) model consists of five process submodels representing the gradual degradation of barriers comprising a nuclear waste package. These processes include radiation, heat, mechanistic, corrosion and leaching, all of which are affected by internal repository and/or external factors. The leach model calculates the mass of matrix and specific nuclides leached from the waste form and accounts for transport of radionuclides in the waste package (diffusion, retardation and advection in the backfill), solubility limits and outputs radial radionuclide concentrations and mass fluxes.
Review Reference:	CEC
Documentation:	INTERA Environmental Consultants Inc., 1982. WAPPA: A Waste Package Performance Assessment Code. Volumes 1-3. SCEPTER Documentation and User's Manual. Prepared by Arthur D. Little, Inc., Cambridge, MA.

GEOCHEMICAL

MODEL SUMMARIES

ARDISC

Model Type: Geochemical/Saturated Ground Water Transport

Author: R.D. Strickert, A.M. Friedman and S. Fried
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Sponsoring Agency: USDOE

Description: The Argonne Dispersion Code (ARDISC) simulates the migration of nuclides through porous media including first-order kinetic adsorption/desorption behaviour. Adsorption rates may differ from desorption rates. Input data in addition to adsorption/desorption rates include equilibrium surface absorption coefficients flow rates, volumes and media porosities. The model has received limited validation through application to a laboratory study.

Review Reference: SAI, CEC

Documentation: Rickert, P.G., R.G. Strickert, and M.G. Seitz. Nuclide Migration in Fractured or Porous Rock, NTIS, PC A03/MF A-1. Argonne National Laboratory, Argonne, IL, p. 28.

Strickert, R.D., A.M. Friedman, S. Fried, 1979. ARDISC (Argonne Dispersion Code): Computer Programs to Calculate the Distribution of Trace Element Migration in Partially Equilibrating Media, ANL-79-25, Argonne National Laboratroy, Argonne, IL, April.

BIOSSIM

Model Type:	Geochemical
Author:	David Garfinkel Moore School of Electrical Engineering University of Pennsylvania Philadelphia, PA 19104
Sponsoring Agency:	National Institute of Health
Description:	BIOSSIM (Biological Structured Simulator) calculates the chemical concentrations in a chemical system as a function of time. Input parameters include a description of the chemical reactions of the system, reaction rate constants and initial chemical concentrations. The code uses this information to generate differential equations describing the time rate of change of the chemical concentrations in accordance with the mass action law. These equations are solved by numerical integration using a predictor corrector method.
Review Reference:	SAI, CEC
Documentation:	Garfinkel, D., 1968. A Machine-Independent Language for the Simulation of Complex Chemical and Biochemical Systems, Computers and Biomedical Research, Vol. 2, pp. 31-44. Garfinkel, D., 1976. BIOSSIM: A Biochemical Simulation Structure System, Moore School of Electrical Engineering Report, University of Pennsylvania, Philadelphia, PA, August. Roman, G.C., and D. Garfinkel. BIOSSIM: A Structured Machine-Independent Biological Simulation Language, Computers and Biomedical Research, Vol. 12, p.3. Roman, G.C. Garfinkel, D. and C.B. Marbach, 1976. Memory Concerning Efficient Methods for Solving Large Sets of Stiff Differential Equations, AFIPS Conference Proceedings, Vol. 45, National Computer Conference, pp. 973-978.

EQ3/EQ6

Model Type: Geochemical

Author: T.J. Wolery
Lawrence Livermore Laboratory
Livermore, CA 94550

Sponsoring Agency: USDOE

Description: EQ3/EQ6 is comprised of two principal programs EQ3 and EQ6. EQ3 computes the distribution of chemical species for an aqueous solution. The program calculates the concentration and thermodynamic activity of all chemical species, ions, ion pairs and complexes in the solution. The program also calculates the saturation state of the fluid for all mineral phases in the data base. EQ6 uses the results of EQ3 to perform reaction path/kinetic simulations for either a closed or flow-through system. The code uses a Newton Raphson method to solve the alebraic governing equations of chemical equilibrium. Output from EQ6 includes the composition of the fluid (distribution of species, pH and Eh), identities and masses of secondary phases absolute and relative rates of irreversible reactions as a function of time and reaction progress.

Review Reference: EPRI, SAI, CEC

Documentation: Wolery, T.J., 1979. Calculation of Chemical Equilibrium Between Aqueous Solution and Minerals: The EQ3/EQ6 Software Package, UCRL-52658, Lawrence Livermore Laboratory, Livermore, CA.

FASTPATH

Model Type: Geochemical

Author/Contact: John A. Apps
Building 90, Room 1140
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

Sponsoring Agency: Kennecott Copper Corporation

Description: FASTPATH simulates the chemical evolution of a chemical system with water present as a function of the reaction process. The code calculates aqueous species, solid phases in thermodynamic equilibrium and the reactants consumed as a function of time. The model operates at a range of discrete temperatures and requires user specified initial aqueous phases and reactant phases.

Review Reference: SAI, CEC

Documentation: Helgeson, H.C., T.H. Brown, A. Nigrini, T.A. Jones, 1972. Calculation of Mass Transfer in Geochemical Processes Involving Aqueous Solutions, Geochimica et Cosmochimica Acta, Vol. 34, pp. 569-592.

GARD

Model Type: Geochemical, Solute Transport

Author: E.L.J. Rosinger and K.K.R. Tremaine
Atomic Energy of Canada Ltd.
Pinawa, Manitoba
ROE 1L0

Sponsoring Agency: Atomic Energy of Canada Ltd.

Description: GARD (Geochemical Assessment of Radionuclide Disposal) uses analytical solutions to one dimensional radionuclide transport equations to simulate the movement of radionuclides from a deep underground disposal vault to the near surface environment. Processes considered include convection, sorption, ion exchange, precipitation and radioactive decay/generation for a three member chain. Dispersion is not considered.

Review Reference: CEC, SAI

Documentation: Rosinger, E.L.J., and K.K.R. Tremaine, 1978. GARD - A Computer Program for the Geochemical Assessment of Radionuclide Disposal, AECL-6318, Atomic Energy of Canada Limited Report.

GEOCHEM

Model Type: Geochemical

Author: G. Sposito and S.V. Mattigod
Department of Soil and Environmental Science
University of California
Riverside, CA 92521

Sponsoring Agency: Kearny Foundation of Soil Science
USDOE, USEPA

Description: The model is a modified version of MINEQL/REDEQL2 that contains many more critically selected data for thermodynamic properties of soils. It contains a method for calculating cation exchange and can correct for up to 3 molal of non-zero ionic strength.

Review Reference: EPRI

Documentation: Sposito, G., and S.V. Mattigod, 1980. GEOCHEM: A Computer Program for the Calculation of Chemical Equilibria in Soil Solutions and Other Natural Water Systems. Kearny Foundation, University of California, Riverside, California.

GROVE/GALERKIN

Model Type:	Geochemical/Ground Water Transport
Author:	David B. Grove U.S. Geological Survey Water Resources Division Mail Stop 413, Box 25046 Denver Federal Center Denver, CO 80225
Sponsoring Agency:	USGS
Description:	This model solves the mass transport equations for an unreactive conservative solute (chloride), a solute with a first-order irreversible rate reaction, radioactive decay and a solute with equilibrium-controlled ion exchange. The model uses a Galerkin finite-element method to solve the mass-transport equations of the solutes in a porous medium.
Review Reference:	SAI, CEC
Documentation:	Grove, D.B.. The Use of Galerkin Finite-Element Methods to Solve Mass-Transport Equations, Water Resources Investigation 77-49. U.S. Geological Survey, Water Resources Division, Denver, CO.

LEVINE

Model Type: Geochemical

Author: H. Levine and D. Miller
Lawrence Livermore Laboratory
Livermore, CA 94550

Sponsoring Agency: USDOE

Description: This model calculates the thermodynamic equilibrium condition for chemical and geochemical systems. The program uses the equilibrium constant approach, allowing a large number of solids, more than one liquid and possibly more than one gas phase to be considered. The program allows for the addition of mass to and the removal of water from the system.

Review Reference: SAI, CEC

Documentation: not available

GTC

MINEQL/REDEQL2

Model Type:	Geochemical
Author:	J. Westall, J. Zachary and F. Morel Department of Civil Engineering Massachusetts Institute of Technology Cambridge, MA 02139
Sponsoring Agency:	Unknown
Description:	This model calculates the chemical equilibrium composition of aqueous systems by solving for mass balances of the components in terms of free component concentrations. Outputs from the code can include absolute concentration of the dissolved species, partitioning and mass transfer between aqueous and non-aqueous phases. The species can include dissolved complexes, gases, solids and redox equilibria.
Review Reference:	CEC, SCEPTER, SAI
Documentation:	Westall, J., J. Zachary and F. Morel, 1976. MINEQL, A Computer Program for the Calculation of Chemical Equilibrium Composition of Aqueous Systems.

MMT

Model Type: Geochemical/Ground Water Transport

Author: S.W. Ahlstrom, H.P. Foote and R.J. Serne
Pacific Northwest Laboratory
Water and Land Resources Department
Richland, WA 99352

Sponsoring Agency: USDOE

Description: MMT simulates the movement of radionuclides and other contaminants in saturated and partially saturated porous media. The model combines contaminant porous media interactions, such as adsorption, ion exchange, precipitation and dissolution, with the results of ground water flow models. The model solves the mass transport problem using a discrete-parcel-random-walk method and simulates dispersion using a random walk analogy. The soil-waste reactions are assumed to be rapidly equilibrating and the resulting system of equations is solved using a simultaneous Newton-Raphson algorithm.

Review Reference: SAI, CEC, EPRI

Documentation: Ahlstrom, S.W., H.P. Foote, R.C. Arnett, C.R. Cole and R.J. Serne, 1977. Multicomponent Mass Transport Model: Discrete-Parcel-Random-Walk Version Theory and Numerical Implementation, BNWL-2127, Battelle Pacific Northwest Laboratories, Richland, WA, May.

Washburn, J.F., et al, 1980. Multicomponent Mass Tranpsort (MMT) Model: A Model for Simulating Migration of Radionuclides in Ground Water, PNL-3179, Pacific Northwest Laboratory, Richland, WA.

PHREEQE

Model Type: Geochemical

Author: D.L. Parkhurst, D.C. Thorstenson, L.M. Plummer
U.S. Geological Survey
Water Resources Division
12201 Sunrise Valley Drive
Reston, VA 22092

Sponsoring Agency: USGS

Description: PHREEQE (pH-REdox-EQuilibrium Equations) is a mass transfer model that can also solve for pH and redox potential as a function of reaction progress. Its aqueous speciation conceptual model is one of ion association with all species and reactions being user defined. The code can be used to calculate mass transfer resulting from the addition of reactants to a solution, titration and or mixing of two waters. Output includes aqueous speciation, including pH and oxidation state of starting solutions and each subsequent solution resulting from any mixing or mass transfer.

Review Reference: NRC, CEC, SCEPTER, EPRI

Documentation: Parkhurst, D.L., D.C. Thorstenson, and L.M. Plummer. U.S. Geological Survey Water Resources Investigation 80-96, NTIS Accession No. PB81 167801, November 1980.

WATEQ/WATEQF

Model Type:	Geochemical
Author:	A.H. Truesdell and B.F. Jones U.S. Geological Survey Washington, DC 20560
Sponsoring Agency:	USDOD
Description:	WATEQ/WATEQF simulates the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original program WATEQ was coded in PL/1 while a similar version WATEQF was coded in Fortran. The program does not provide a complete description for the processes leading up to the equilibrium distribution, it can indicate which processes are impossible, which process may control water composition and processes which are controlled by kinetic factors.
Review Reference:	CEC, NRC, SAI, EPRI
Documentation:	1974. WATEQ, A Computer Program for Calculating Chemical Equilibria of Natural Waters, Journal of Research -- U.S. Geological Survey, Vol. 2, No. 2, March-April, pp. 233-248.

UNSATURATED GROUND WATER FLOW

MODEL SUMMARIES

Table 1. Capabilities of Unsaturated Ground Water Flow Models

Model	Dimensionality	Time[1] Dependence	Solution[2] Technique	Boundary Conditions	Comments
COLORADO FD	3		FD		
FEMWATER	2	T	FE	Head, Flux	Areal, Vertical Plumes
FREEZE	3	T	FD		Saturated, Unsaturated
INTERCOMP-GWM	3	T	FD		Two-Phase
KANSAS-GREEN	2		FD		Multi-Phase
PST			FD		
REEVES-DUGUID	2	T	FE		
UNSAT2	2	T	FD	Head, Flux	Areal, Vertical, Radial

[1] SS = Steady State: T = Transient

[2] FD = Finite Difference: FE = Finite Element

COLORADO-FD

Model Type: Unsaturated Ground Water Flow

Author: W. F. Brutsaert and C. Way

Sponsoring Agency: Unknown

Description: Originally this model was restricted to two-dimensional flow systems but it has since been expanded to three. The model uses upstream weighting of the capillary conductivity in its finite difference formulation and solves the resulting equations using Newton's iterative technique. The model has been applied to a 40 mile reach of the Arkansas River in Colorado.

Review Reference: SAI, EPRI

Documentation/ Reference : Brutsaert, W. F., 1971. A Functional Iteration Technique for Solving the Richards Equation Applied to Two-Dimensional Infiltration Problems, Water Resources Research, Vol. 7, No. 6, pp. 1583-1595.

Brutsaert, W., and C. Way, 1973. A Conjunctive Use Surface Water-Groundwater Simulator, New Mexico Water Resources Research Institute Partial Technical Completion Report No. 033, November.

GTC

FEMWATER

Model Type: Unsaturated Ground Water Flow

Author:
G. T. Yeh
Oak Ridge National Laboratory
Bldg. 1505, Rm 203
P. O. Box X
Oak Ridge, TN 37830

D. S. Ward
INTERA Environmental Consultants, Inc.
11511 Katy Freeway, Suite 630
Houston, TX 77079

Sponsoring Agency: USDOE

Description: This is a two-dimensional finite element model capable of simulating the ground water flow in saturated-unsaturated systems. This model is an extension of the Duguid-Reeves code also developed at ORNL. The Duguid-Reeves approach to calculating the flow field leads to a discontinuous velocity field which can significantly affect the accuracy of subsequent mass transport modeling. FEMWATER incorporates a technique to overcome this problem resulting in a continuous velocity field. Necessary inputs to the model include initial head distributions, prescribed head and flux boundary conditions, hydraulic conductivities, storage coefficient and material non-linearities. The model can simulate either an areal plane or vertical cross-section.

Review Reference: NRC, EPRI

Documentation/Reference: Yeh, G. T., 1982. Training Course No. I: The Implementation of FEMWATER (ORNL-5567) Computer Program. ORNL/TM-8327, NUREG/CR-2705, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

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Yeh, G. T. and D. W. Ward, 1980. FEMWATER: A Finite Element Model of Water Flow Through Saturated Unsaturated Porous Media. ORNL-5567, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Yeh, G. T., 1983. FEMWATER-1: A Finite Element Model of Water Flow through Saturated-Unsaturated Porous Media - First Revision. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

FREEZE

Model Type: Unsaturated Ground Water Flow

Author: R. A. Freeze
University of British Columbia
Vancouver, B.C.

Sponsoring Agency: IBM

Description: This model is a three-dimensional finite difference code developed to simulate transient saturated-unsaturated flow in heterogeneous geologic basins. The model can be applied to both confined and unconfined saturated aquifers and provides quantitative hydrographs of surface infiltration, ground water recharge, water table depth and stream base flow. The model uses a line successive over-relaxation (LSOR) technique to solve the integrated flow equations.

Review Reference: SAI

Documentation/ Reference : Freeze, R. A., 1971. Three-Dimensional Transient Saturated-Unsaturated Flow in a Ground Water Basin, Water Resources Research, Vol. 7, No. 2, pp 347-366.

INTERCOMP-GWM

Model Type: Unsaturated Ground Water Flow

Author: K. H. Coats
Intercomp Resource Development Services
Houston, Texas

Sponsoring Agency: Unknown

Description: Intercomp GWM (Gas Water Model) is a three-dimensional model describing the simultaneous flow of water and air (i.e., multiphase model). The two fluids are assumed immiscible but either can saturate the flow system. The model uses either a line successive over-relaxation technique or a direct Gaussian elimination (used in conjunction with a special ordering scheme) to solve the finite difference approximations to the partial differential equations. There are two versions of the model, one which uses an implicit pressure/explicit saturation (IMPES) approach, the other a completely simultaneous solution of the pressures and saturations. The latter can incur approximately 50 to 100% more in computer costs.

Review Reference: SAI

Documentation/ Reference : None Reported

KANSAS-GREEN

Model Type:	Unsaturated Ground Water Flow
Author:	D. W. Green Kansas Water Resources Research Institute Manhattan, Kansas 66502
Sponsoring Agency:	Unknown
Description:	This is a multiphase model which addresses the flow of both water and air in porous media. The model is a two-dimensional finite difference model which solves the systems of equations using an alternating direction implicit (ADI) method.
Review Reference:	SAI
Documentation/ Reference :	Green, D. W. et al., 1969. Numerical Modeling of Unsaturated Groundwater Flow, Contrib. 31, Kansas Water Resources Research Institute, Manhattan, KS. Green, D. W. et al., 1970. Numerical Modeling of Unsaturated Groundwater Flow and Comparison of the Model to a Field Experiment, Water Resources Research, Vol. 6, No. 3, pp. 862-874.

PST

Model Type: Unsaturated Ground Water Flow

Author: A. E. Reisenauer, D. B. Cearlock
and C. A. Bryan
Battelle Pacific Northwest Laboratories
Richland, WA 99352

Sponsoring Agency: USDOE

Description: The PST (Partially Saturated Transient) model can simulate unsaturated fluid flow in heterogeneous porous media. The model uses an unspecified iterative technique to obtain a solution to finite difference approximations. The model is restricted to use in isothermal conditions and has been described as being computationally slow.

Review Reference: SAI

Documentation/ Reference : Reisenauer, A. E., D. B. Cearlock, and C. A. Bryan, 1975. BNWL-1713, Battelle Pacific Northwest Laboratories, Richland, WA

REEVES-DUGUID

Model Type: Unsaturated Ground Water Flow

Author: M. Reeves and J. O Duguid
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: NSF

Description: This model calculates saturated and unsaturated ground water flow in a two-dimensional system. The model uses a finite element method for spatial integration and a centred in time finite difference approximation. The non-linear capillary conductivity and saturation are calculated by cyclic solution of the pressure heads. Stability problems using this approach have been encountered at low moisture contents. The Reeves-Duguid model is affiliated to the Duguid-Reeves code which does contaminant transport for the same system using the calculated flow velocities.

Review Reference: CEC, SAI

Documentation/ Reference : Reeves, M., and J. O. Duguid, 1975. Water Movement Through Saturated-Unsaturated Porous Media: A Finite-Element Galerkin Model, ORNL-4927, Oak Ridge National Laboratory, Oak Ridge, TN.

UNSAT2

Model Type: Unsaturated Ground Water Flow

Author: UNSAT2 was developed by S. P. Neuman, R. A. Feddes, and E. Bresler. The primary contact in the United States is:

Shlomo P. Neuman
Department of Hydrology and Water Resources
University of Arizona
Tucson, AZ 85717

Sponsoring Agency: U. S. Department of Agriculture
Project No. ALO-SWC-77

Description: This model describes the transient flow of water in a saturated/unsaturated porous media. The model can be used for both areal and vertical cross-sections as well as radial systems. The model uses a finite element method and a fully implicit iterative algorithm to obtain solutions to the unsaturated flow equations. Input variables include initial head (or pressure) distribution, rates of infiltration, evaporation and transpiration, hydraulic conductivity tensor, relative permeability function, capillary pressure function and storage coefficient. Output from the model consists of an echo of input data, material properties, boundary types, total head values, pressure head values, moisture contents and discharge rates into or out of the system. A wide variety of time-dependent boundary conditions may be prescribed including pressure head, flux, seepage faces, evaporation and infiltration.

Review Reference: EPRI, SAI, CEC

Documentation/ Reference: Neuman, S. P., R. A. Feddes and E. Bresler, 1974. Finite Element Simulation of Flow in Saturated-Unsaturated Soils Considering Water Uptake by Plants, Third Annual Report. Project ALO-SWC-77, Hydrodynamics and Hydraulic Engineering Laboratory Technician, Haifa, Israel.

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Feddes, R. A., S. P. Neuman and E. Bresler, 1975. Finite Element Analysis of Two-Dimensional Flow in Soils Considering Water Uptake by Roots: II. Field Applications. Soil Science Society of America Proceedings, Vol. 3, No. 3, pp. 231-237.

Feddes, R. A., E. Bresler and S. P. Neuman, 1974. Field Test of a Modified Numerical Model for Water Uptake by Root Systems. Water Resources Research, Vol. 10, No. 6, pp. 1199-1206.

Feddes, R. A. and M. G. van Steenberger, 1973. Subirrigation Field 'de Groeve. Nota 735, Inst. for Land and Water Management Res., Wageningen, The Netherlands (in Dutch)

SATURATED GROUND WATER FLOW

MODEL SUMMARIES

Table 2. Capabilities of Saturated Ground Water Flow Models

Model	Dimensionality	Time[1] Dependence	Solution[2] Technique	Boundary Conditions	Comments
BEWTA	2	T	FD		Phreatic
BRINE	1	T			Density Dependent Flow
COOLEY	2	T	FE		Confined, Unconfined
ESOPH	2	T	FD		Leaky Aquifer
FEGWM	2		FE	Head	Confined, Unconfined
FE3DGW	3	T	FE	Head, Flux	
FLOP1, FLOP2 FRONT-N	1	T	Rurge Kuta		One dimensional stream line solutions
FREESURF I & II	2	SS(I), T (II)	FE		Cross-sections, axisymmetric
GABHYD	Quasi 3	T	FD		2D systems connected by leakage
GWATER			FD		
LM4	2	SS	FE	Head, Flux	

Table 2. Capabilities of Saturated Ground Water Flow Models (cont'd)

Model	Dimensionality	Time[1] Dependence	Solution[2] Technique	Boundary Conditions	Comments
MTMVMC	Quasi 3		FD	Head, Flux	2D systems connected by leakage
NETFLO	1D Systems				Series of Stream Tubes
P1	2		FD	Head, Flux	
RCPIGW	2		Analytic		
SATUNA	2				Saturated, Unsaturated
SHIBASAKI 1,2,3	2, Quasi 3	T	FD		Considers Consolidation
SUPERMOCK	2	T			Saturated, Unsaturated
USGS2D	2	T	FD		Phreatic
USGS3D	3	T	FD		Phreatic
VTT	Quasi 3	T, SS	FD	Head, Flux	Confined, Unconfined
V3	2	T	FD	Constant Head, Flux	Confined

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[1] SS = Steady State: T = Transient

[2] FD = Finite Difference: FE = Finite Element

BEWTA

Model Type: Saturated Ground Water Flow Model

Author: Dr. Chang L. Lin
N.S. Department of the Environment
P.O. Box 2107
Halifax, Nova Scotia

Sponsoring Agency: Unknown

Description: The model solves the transient equation of ground water flow for a phreatic aquifer (Boussinesq equation) in a horizontal plane (two dimensional). The equation is approximated by a finite difference equation and is solved using an alternating direction implicit method. Principal assumptions include Dupuit assumptions for a phreatic aquifer, constant fluid density and negligible contribution from the unsaturated zone. Aquifer parameters can be slightly anisotropic and non-homogeneous.

Review Reference: SAI

Documentation/ Reference : Not available

BRINE

Model Type: Saturated Ground Water Flow Model

Author: M. E. Fuller
Lawrence Livermore Laboratory
Livermore, CA 94550

Sponsoring Agency: Unknown

Description: The model calculates the brine migration in ground water near a nuclear waste canister in a hidden salt repository. The program calculates the one-dimensional brine velocity at various times and points from the centre of a cylindrical canister. The model accounts for diffusion, density variability and thermal gradients. The spatial temperature distribution as a function of time must be input into the model.

Review Reference: SAI, CEC

Documentation/Reference: C. D. Duckworth and M. E. Fuller, 1980. BRINE: A Computer Program to Compute Brine Migration Adjacent to a Nuclear Waste Canister in a Salt Repository, NTIS, UCID 18666.

COOLEY

Model Type:	Saturated Ground Water Flow Model
Author:	R. L. Cooley U. S. Geological Survey Water Resources Division Box 25046, Stop 413 Denver Federal Centre Denver CO 80225
Sponsoring Agency:	USGS
Description:	This model calculates the hydraulic head distribution and velocity field in a confined, semi-confined or unconfined aquifer. Flow may be either transient or steady. Aquifer representation is limited to 2-dimensional planar (cross-sectional or areal) or radial. Aquifer parameters may be distributed or zoned, and anisotropic assuming principal permeability axis coincides with the system co-ordinate axis. Leakage from the confining bed is assumed vertical while storage in this layer is neglected. The Dupuit-Forcheimer assumptions together with a delayed (or non-delayed) yield concept form the basis for the water table case in plan view. The systems of equations are solved using a finite element method with the time discretized by a weighted average technique. The code has been verified against four problems to which analytical solutions are available and has been applied to a number of field problems.
Review Reference:	SAI, CEC, NRC
Documentation/ Reference :	R. L. Cooley, 1974. Finite Element Solutions for the Equations of Groundwater Flow, Technical Report Series H-W, Hydrology and Water Resources Publication No. 18, Center for Water Resources Research, Desert Research Institute, University of Nevada System, Reno.

ESOPH

Model Type: Saturated Ground Water Flow Model

Author: Dr. A. Vanderberg

Sponsoring Agency: Environment Canada

Description: ESOPH calculates the transient piezometric head distribution in a single leaky aquifer using a finite difference approximation to the flow equation. The model solves the resulting system of equations using an alternating direction implicit technique. The aquifer can contain a number of wells for both recharge and discharge.

Review Reference: SCEPTER

Documentation/ Reference : N/A

GTC

FEGWM

Model Type:	Saturated Ground Water Flow Model
Author:	R. T. Hurr Colorado District Water Resources Div. U.S.G.S. Denver CO
Sponsoring Agency:	USGS
Description:	The model was designed for application to a single layered aquifer (i.e., 2-D horizontal system). The model can be used to predict potentiometric head and recharge/discharge from constant head boundaries in either a confined or unconfined system. Media may be anisotropic and non-homogeneous on an element-by-element basis. Recharge may be either point or areally distributed. The model uses a finite element method and solves the resulting system of equations by Gaussian elimination.
Review Reference:	SCEPTER, WISAP
Documentation/ Reference:	Not reported.

GTC

FE3DGW

Model Type: Saturated Ground Water Flow Model

Author: Gupta, S. K., C. R. Cole and F. W. Bond

Sponsoring Agency: Battelle Pacific Northwest Laboratories

Description: This model is a three-dimensional finite element code for describing a transient saturated ground water flow. Source/sink terms may be either point, linear or areal. Pumping stresses may be described as a function of time. Boundary elements may be either prescribed pressure or prescribed flux. All parameters (hydraulic conductivity and specific storage) may be heterogeneous with hydraulic conductivity being anisotropic as well. Output from the model consists of heads and velocity vectors at a node after every time step. Auxiliary programs have been developed to plot grid values, contour maps and three-dimensional charts of both the input data and the results.

FE3DGW has only been used extensively by PNL. The reason for this is the machine dependence of the existing software. The model was developed on and optimized to run on a PDP-11/45.

Review Reference: CEC, NRC, SCEPTER

Documentation/Reference: C. R. Cole and S. K. Gupta, 1979. A Brief Description of the Three-Dimensional Finite Element Ground-Water Flow Model Adapted for the Waste Isolation Safety Assessment Program. Report PNL-2652, Pacific Northwest Laboratory, Richland, WA.

S. K. Gupta, C. R. Cole and F. W. Bond, 1980. Finite Element Three-Dimensional Groundwater (FE3DGW) Flow Model - Formulation, Program Listings and Users' Manual. Report PNL-2939, Pacific Northwest Laboratory, Richland, WA.

FLOP1, FLOP2, FRONT-N

Model Type:	Saturated Ground Water Flow Model
Author:	C. van den Akker Municipal Waterworks of Amsterdam Condensatorweg 54 Amsterdam - Stoterdijk
Sponsoring Agency:	Unknown
Description:	These models calculate streamlines and residence times for water particles in a homogeneous aquifer. The aquifer is assumed to be infinite and horizontal and may contain pumping or injection wells. Two simultaneous differential equations are solved using the Runge-Kutta method to obtain path lines and flow times. FLOP1 was written for confined aquifers while FLOP2 was written for semi-confined aquifers. Both FLOP1 and FLOP2 assume no storage. FRONT-N is similar to FLOP1 but does consider aquifer storage. Potential head data in the form of analytical functions or tabular data (from measured data or numerical solutions) may be incorporated into the model.
Review Reference:	SAI, WISAP
Documentation/ Reference :	Not reported.

FREESURF I & II

Model Type: Saturated Ground Water Flow Model

Author: S. P. Neuman, P. A. Witherspoon
University of Arizona
Tucson, Arizona 85712

Sponsoring Agency: Unknown

Description: These models were developed to calculate piezometric heads and flow rates in a heterogeneous and anisotropic media under steady (FREESURF I) and transient (FREESURF II) conditions. The model can accommodate both confined and free-surface systems by virtue of finite elements that can expand or contract to accommodate the location of the water table. The program can also determine the existence of a seepage face through a two-step iterative procedure. The models are two-dimensional or axisymetric and restricted to vertical sections when the free-surface feature is used.

Review Reference: SAI, SCEPTER, WISAP

Documentation/ Reference: Neuman, S. P. and P. A. Witherspoon, 1972. FREESURF I - A Finite Element Computer Program for Two Dimensional and Axisymetric Steady Flow of Groundwater with a Free Surface. Dept. of Civil Engineering, University of California, Berkeley, CA.

GABHYD

Model Type:	Saturated Ground Water Flow Model
Author:	G. E. Seidel Bureau of Mineral Resources, Geology & Geophysics CUS Constitution Canberra, ACT 2601, Australia
Sponsoring Agency:	Unknown
Description:	This model was developed expressly for the purpose of predicting heads and free-flowing well discharges in the Great Artesian Basin, Australia. The model represents each confined aquifer by a single two-dimensional layer with individual layers connected solely by leakage. The uppermost aquifer is maintained at constant head while side boundaries are either no flow or prescribed pressure. Aquifers are assumed to be fully saturated while compressibilities are represented by storativities. Aquifers may be non-homogenous and anisotropic. The equations representing ground water flow are approximated by a finite difference formulation and solved using a Gauss-Seidel iterative technique. Time differencing is fully implicit.
Review Reference:	WISAP
Documentation/ Reference :	Not reported.

GWATER

Model Type:	Saturated Ground Water Flow Model
Author:	D. Kelinecke P. O. Box 3012 Santa Barbara, CA
Sponsoring Agency:	Unknown
Description:	Little information is available regarding this model. It is known that it simulates saturated ground water flow using a finite difference approximation and solves the resulting equation by Gauss-Seidel iteration.
Review Reference:	WISAP, SCEPTER
Documentation/ Reference :	None reported.

LM4

Model Type: Saturated Ground Water Flow Model

Author: A. Verruijt
University of Technology
Delft, Netherlands

Sponsoring Agency: Unknown

Description: This model can be used to predict the steady-state head distribution in a two-dimensional aquifer system. Boundary conditions include prescribed head or prescribed flux. Interior sources/sinks can be incorporated into the grid. The code uses a finite element method solving linear systems of equations using a Gauss-Seidel iterative technique.

Review Reference: WISAP, SCEPTER

Documentation/Reference: Not reported.

MTMVMC

Model Type:	Saturated Ground Water Flow Model
Author:	A. Carriere GERSAR Nimes, France
Sponsoring Agency:	Unknown
Description:	This model can be used to predict piezometric heads in a multi-layered aquifer. The individual layers are two-dimensional with leakage between adjacent layers assumed to be vertical. The aquifer can be either phreatic (using the Dupuit approximation) or confined. Boundary conditions may be either prescribed flux or head. The flow equation is represented by a finite difference approximation and solved by an over-relaxation method. The code is unavailable.
Review Reference:	WISAP, SCEPTER
Documentation/ Reference :	Unknown

NETFLO

Model Type:	Saturated Ground Water Flow Model
Author:	INTERA Environmental Consultants Inc. 11999 Katy Freeway Houston, TX 77079
Sponsoring Agency:	USDOE
Description:	This model simulates ground water flow through a system of equivalent one-dimensional ducts connected both in series and in parallel. The code is based upon the principle of conservation of mass at a node together with Darcy's Law. Output consists of the pressure and flow rate in each segment.
Review Reference:	CEC
Documentation/ Reference :	INTERA Environmental Consultants, Inc., 1982. NETFLO - A Network Ground-Water Flow Code. SCEPTER Documentation and User's Manual. ONWI/E512-02900/CD-01, Office of Nuclear Waste Isolation.

GTC

P1

Model Type:	Saturated Ground Water Flow Model
Author:	T. A. Prickett Illinois State Water Survey Box 232 Urbana, Ill. 61801
Description:	The model predicts head distribution in a two-dimensional leaky or confined aquifer. Aquifer properties may be heterogeneous and anisotropic. Boundary conditions may be either constant head or constant flow. The model solves a finite difference approximation to the flow equation using a modified ADI scheme.
Review Reference:	WISAP, SCEPTER
Documentation/ Reference :	Not reported.

RCPIGW

Model Type: Saturated Ground Water Flow Model

Author: D. B. McWhorter
Dept. of Agricultural Engineering
Colorado State University
Fort Collins, CO 80523

Description: The model solves analytic expressions for the flow equations in a two-dimensional aquifer. The model describes a saturated homogeneous, isotropic aquifer and a homogeneous incompressible fluid.

Review Reference: BNWL

Documentation/Reference: Unknown

SATUNA

Model Type:	Saturated Ground Water Flow Model
Author:	P. Huyakorn Geotrans Inc. Reston, VA 22090
Description:	This model calculates flow in a saturated or unsaturated porous media and couples the influence of temperature. The code is proprietary and is not available to the general public.
Review Reference:	SAI
Documentation/ Reference :	N/A

SHIBASAKI 1, -2, -3

Model Type:	Saturated Ground Water Flow Model
Author:	Tatsuo Shibasaki Fujigane 182 Tsurugashima Saitama 350-02
Sponsoring Agency:	Unknown
Description:	Shibasaki 1 calculates the piezometric head decline in a two-dimensional confined aquifer with or without leakage. Shibasaki 2 calculates the piezometric head change in a vertical cross-section and the compression (land subsidence) in deep strata. Shibasaki 3 is a quasi three-dimensional two-aquifer model which can be used to predict piezometric head decline and land subsidence. All three models solve a finite difference approximation to the flow equation by an ADI technique.
Review Reference:	WISAP, SCEPTER
Documentation/ Reference :	None reported.

SUPERMOCK

Model Type: Saturated Ground Water Flow Model

Author: M. S. Bedinger
USGS
Lakewood, CO 80225

Sponsoring Agency: USGS

Description: This model was specifically developed to simulate the transient water table response and piezometric heads in an unsaturated aquifer system in the Red River Valley in Lousianna. The model simulates two-dimensional (horizontal) flow in the saturated aquifer, one-dimensional flow in an overlying fine-grained strata and soil moisture in the unsaturated zone.

Review Reference: WISAP

Documentation/ Reference : N/A

USGS2D

Model Type: Saturated Ground Water Flow Model

Author: P. C. Trescott
U. S. Geological Survey
Reston, Virginia 22092

Sponsoring Agency: USGS

Description: This model is capable of calculating the piezometric head in a two-dimensional aquifer which may be either (or both) water table or artesian. USGS2D has numerous options regarding ground water flow conditions, source terms and numerical solution techniques. These include the existence of a line successive over-relaxation method, or an iterative alternating direction implicit method or a strongly implicit method, all of which can be used to solve the finite difference appproximations. Model options pertaining to the ground water system include leakage (steady or transient) from confining beds (in which effects of storage are considered), recharge, pumping wells and evapotranspiration. The model was originally intended to be applied to areal planar aquifers but has been applied to vertical cross-sections.

Review Reference: CEC, EPRI, NRC

Documentation/ Reference:

P. C. Trescott, G. F. Pinder and S. P. Larson, 1976. Finite-Difference Model for Aquifer Simulation in Two dimensions with Results of Numerical Experiments. U.S. Geological Survey, Techniques of Water-Resources Investigations, Book 7, Chapter C1.

S. P. Larson (1979). Direct Solution Algorithm for Two Dimensional Ground-Water Flow Model. U. S. Geological Survey Open File Report 79-202.

USGS3D

Model Type: Saturated Ground Water Flow Model

Author:
P. C. Trescott
U. S. Geological Survey
Reston, Virginia 22092

Sponsoring Agency: USGS

Description: This model can simulate transient ground water flow in either a fully three-dimensional or a quasi three-dimensional mode. The uppermost layer may be phreatic in nature and subject to recharge. The medium may be anisotropic and heterogeneous and have irregular boundaries. If it is reasonable to neglect storage and horizontal flow within confining layers, the effect of vertical leakage can be incorporated into the vertical anisotropy of adjacent aquifers. The model does assume constant fluid density, viscosity and temperature. This model is widely accepted.

Review Reference: CEC, NRC

Documentation/ Reference :

P. C. Trescott, 1975. Documentation of Finite-Difference Model for Simulation of Three-Dimensional Ground-Water Flow. U.S. Geological Survey Open-File Report 75-438.

P. C. Trescott and S. P. Larson, 1976. Supplement to Open-File Report 75-438. U.S. Geological Survey Open-File Report 76-591.

VTT

Model Type: Saturated Ground Water Flow Model

Author: A. E. Reisenauer
Pacific Northwest Laboratory
Richland, WA 99352

Sponsoring Agency: USDOE

Description: This model calculates the piezometric head distribution in confined or unconfined aquifers with provision for inter-aquifer transfer through the use of transfer coefficients. Boundary conditions are variable and consist of prescribed head, flux or no flow boundaries. The model uses a finite difference method to approximate the flow equation. The resulting equations are solved using either a direct Gaussian elimination procedure in conjunction with Newton's method or a Cholesky decomposition for the steady-state case and a line successive over-relaxation method for transient solutions.

Review Reference: CEC, NRC

Documentation/Reference: A. E. Reisenauer, 1979. Variable Thickness Transient Groundwater Flow Model, Vol. 1, Formulation; Vol. 2, User's Manual; Vol. 3, Program Listings. PNL-3160-1,2,3, Pacific Northwest Laboratory.

V3

Model Type: Saturated Ground Water Flow Model

Author: T. A. Prickett and C. G. Lonnquist

Sponsoring Agency: Illinois State Water Survey

Description: This model calculates the piezometric head in a two-dimensional (areal) confined system under transient conditions. The aquifer can be heterogeneous and anisotropic while the fluid is homogeneous. Boundary conditions may consist of either constant head or flux. The model uses a Gauss-Seidel iterative technique to solve finite difference equations.

Review Reference: SCEPTER, V3

Documentation/ Reference : None reported.

SOLUTE TRANSPORT

MODELS

Table 3. Capabilities of Solute Transport Models

Model	Dimensionality	Trace Species	Solution Technique	Flow Field	Comments
AT123D	1,2, or 3	Decay, Adsorption	Analytic	Constant, Uniform	Various Release Mechanisms
AUTOMIG-2A	1	Decay, Adsorption	Analytic	Input	
COFAM	1	Decay, Adsorption	Semi-Analytic	Constant	Used for trenches
DICKMAN	1	Decay	Partially Saturated		
DPRW/MMT	2,1	Decay, Generation (1-D)	DRPW	Input	
DUGUID/REEVES	2	Decay, Adsorption	FE	Input	
FEMWASTE	2	Decay, Adsorption		Input	
FRONT	2	Conservative		Input	
GETOUT	1	Decay, Generation Adsorption	Analytic	Steady, Input	
HCTM	3	Decay, Adsorption (equilibrium and kinetic)	MOC, FD	Saturated	
HYDRO	1	Decay, Adsorption	FD	Unsaturated	
ISOQUAD2, PINDER	2		FE	Steady or Transient	

Table 3. Capabilities of Solute Transport Models (cont'd)

Model	Dimensionality	Trace Species	Solution Technique	Flow Field	Comments
KONBRED/ USGSMOC	2	Non-reactive	FD(flow) MOC (transport)		
NRC LPGS	3		Semi-Analytic	Constant	
NWFT/DVM	1-D Network	Decay, Generation, Adsorption	DVM		
OGRE	1,2				Fully Transient
PATHS	1	Adsorption	Numerical	Steady or Transient	No Dispersion
PCP	2		Semi-Analytic		
PERCOL	1	Adsorption		Steady	
ROBERTSON 2/ INEL TRANSPORT I	2	Decay, Adsorption	Flow-FD Transport-MOC	Transient	
SALTRP	2		FE	Transient	Density Dependent
SEGOL	3		FE	Transient, Steady	Saturated, Unsaturated
STM	1,2		Decay,Adsorption		

Table 3. Capabilities of Solute Transport Models (cont'd)

Model	Dimensionality	Trace Species	Solution Technique	Flow Field	Comments
SWIFT	3	Decay, Generation	FD	Transient	Considers leaching, inventory, dissolution
SWIP	3		FD	Transient or Steady	
TRANSAT	2	Decay, Adsorption	FE	Steady State	
TRENCH		Decay, Adsorption		Input	
UCB-NE-10, UCB-NE-30	1	Decay, Generation, Adsorption	Semi-Analytic		

AT123D

Model Type: Solute Transport

Author: G.T. Yeh
Environmental Sciences Division, Bldg. 1505
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: AT123D provides analytic solutions to the transient solute transport equation in one, two or three dimensions. Various source configurations (point, line, rectangular or rectangular prism) and release rates (instantaneous, band release or step function) are included. Equilibrium adsorption and radioactive decay are considered but decay chains are not. Ground water flow is assumed to be constant and uniform.

Review Reference: ERPI, NRC

Documentation: Yeh, G.T., AT123D: Analytical, Transient, One-, Two-, Three-Dimensional Simulation of Waste Transport in the Aquifer System, Contract No. W-7405-eng-26, Environment Sciences Division Publication No. 1439, Oak Ridge National Laboratory, Oak Ridge, TN.

AUTOMIG-2A

Model Type: Solute Transport

Author/Contact: Robert D. Baird
Ford, Bacon & Davis Utah
375 Chipea Way
Salt Lake City, UT 84108

Sponsoring Agency: USNRC

Description: AUTOMIG-2A solves the one-dimensional transport equation using the analytic solution for point sources in saturated porous media. Release zones and aquifer transport are represented by different pathways. Generation of radioactive isotopes is ignored. Water velocities along pathways are a necessary input.

Review Reference: SAI, CEC

Documentation: Adam, J.A. and V.L. Rogers, 1978. A Classification System for Radioactive Waste Disposal - What Waste Goes Where? NUREG-0456, U.S. Nuclear Regulatory Commission, Washington, DC, July.

COFAM

Model Type: Solute Transport

Author: A.H. Lu
N.Y. State Department of Health
Albany, NY 10221
Salt Lake City, UT 84108

Sponsoring Agency: Health Research Inc.

Description: COFAM is a semi-analytical model originally developed to model the migration of leachate from radioactive waste burial trenches. The model includes the effects of dispersion, adsorption and radioactive decay. Water flux into the trench is assumed constant.

Review Reference: SAI, CEC

Documentation: Lu, A.H., 1978. Modeling of Radionuclide Migration from a Low-Level Radioactive Waste Burial Site, Health Physics, Vol. 34, No.1, pp. 39-44.

DICKMAN

Model Type: Solute Transport

Author: Paul T. Dickman
EG&G Idaho
Box 1625
Idaho Falls, ID 83401
FTS 583-0610

Sponsoring Agency: USDOE

Description: DICKMAN was developed to model the transport of transuranic wastes through soil and basalt. It is a one-dimensional partially saturated code and considers the following transport processes; sorption, precipitation, dissolution and decay.

Review Reference: SAI, CEC

Documentation: Unknown

DPRW/MMT

Model Type: Solute Transport

Author: S.W. Ahlstrom and H.P. Foote
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: DRPW/MMT (Discrete Parcel Random Walk/Multicompnent Transport Model) can be used to calculate the transport of dissolved contaminant in ground water. The model is currently available as either a two-dimensional version that does not consider daughter products or a one-dimensional versions that does consider generation. The model calculates the transport of the radionuclide along a pathline with water velocity, retardation and dispersivity capable of varying along the path. It can model radionuclides as more than one chemical species. The code does only transport simulations and hence requires ground water potentials or velocities as input.

Review Reference: SAI, CEC, IGWMC, NRC

Documentation: Ahlstrom, S.W., and H.P. Foote, 1976. Multicomponent Mass Transport-Discrete Parcel Random Walk Model Theory and Numerical Implementation, BNWL-2127, Battelle Pacific Northwest Laboratories, Richland, WA, December.

GTC

DUGUID REEVES

Model Type: Solute Transport

Author:

J.O. Duguid
Office of Nuclear Waste Isolation
Battelle Memorial Institute
Columbus, OH 4302

M. Reeves
Intera Technologies Inc.
11999 Katy Freeway, Suite 610
Houston, Texas 77079

Sponsoring Agency: USDOE

Description: The DUGUID-REEVES model is a two dimensional solute transport model designed to be coupled to the REEVES-DUGUID saturated/unsaturated ground water flow model. The model uses a Galerkin finite element method to perform the spatial integration while the time integration is performed using a modified Crank-Nicholson finite difference formulation. The model includes the effects of advection, dispersion, and exchange of one chemical component as well as radioactive decay.

Review Reference: SAI, CEC, EPRI

Documentation:

Duguid, J.O. and M. Reeves, 1976. Material Transport Through Porous Media: A Finite Element Galerkin Model, ORNL-49280, Oak Ridge National Laboratory, Oak Ridge, TN, March.

Reeves, M., and J.O. Duguid, 1975. Water Movement Through Saturated-Unsaturated Porous Media: A Finite-Element Galerkin Model, ORNL-4927, Oak Ridge National Laboratory, Oak Ridge, TN.

FEMWASTE

Model Type:	Solute Transport
Author:	G.T. Yeh Environmental Sciences Division, Bldg. 1505 Oak Ridge National Laboratory P.O. Box X Oak Ridge, TN 37830 D.S. Ward GEOTRANS Ino. 201 Elden Street Herndon, Virginia 22070
Sponsoring Agency:	USDOE
Description:	FEMWASTE is a two-dimensional model capable of simulating solute transport through saturated/unsaturated porous media. Transport mechanisms include advection, hydrodynamic dispersion, chemical sorption and radioactive decay. The model may be applied to either cross-sectional or areal systems and requires a velocity field as input.
Review Reference:	NRC, SAI, CEC, EPRI, SCEPTER
Documentation:	Yeh, G.T., and D.S. Ward, 1979. A FEMWASTE Finite-Element Model of Waste Transport Through Saturated-Unsaturated Porous Media, ORNL-5601, Oak Ridge National Laboratory, Oak Ridge, TN.

FRONT

Model Type:	Solute Transport
Author:	A. Vandenberg Inland Waters Directorate Ottawa, Ontario Canada
Sponsoring Agency:	Environment Canada
Description:	FRONT was developed to simulate the movement of an intrusion front in a two-dimensional (horizontal) aquifer. The model predicts the location of a front for a given ground water flow field. The program neglects dispersion at the front interface.
Review Reference:	SAI, CEC
Documentation:	Vandenberg, A.L., 1975. Program FRONT - Simulation of a Moving Intrusion Front in a Thin Horizontal Confined Aquifer, Department of the Environment, Ottawa, Ontario, Water Resources Branch.

GARD

Model Type:	Geochemical, Solute Transport
Author:	E.L.J. Rosinger and K.K.R. Tremaine Atomic Energy of Canada Ltd. Pinawa, Manitoba ROE 1L0
Sponsoring Agency:	Atomic Energy of Canada Ltd.
Description:	GARD (Geochemical Assessment of Radionuclide Disposal) uses analytical solutions to one dimensional radionuclide transport equations to simulate the movement of radionuclides from a deep underground disposal vault to the near surface environment. Processes considered include convection, sorption, ion exchange, precipitation and radioactive decay/generation for a three member chain. Dispersion is not considered.
Review Reference:	CEC, SAI
Documentation:	Rosinger, E.L.J., and K.K.R. Tremaine, 1978. GARD - A Computer Program for the Geochemical Assessment of Radionuclide Disposal, AECL-6318, Atomic Energy of Canada Limited Report.

GETOUT

Model Type: Solute Transport

Author: S.C. Sneider, M.O. Cloninger, and H.C. Burkholder
Battelle Pacific Northwest Laboratory
Battelle Boulevard
Richland, WA 99352

Sponsoring Agency: USDOE

Description: GETOUT solves the solute transport equation for one, two or three member decay chains in a one-dimensional system using analytical solutions. The model includes the effects of adsorption and dispersion. The velocity field is assumed to be steady and saturated and must be specified by the user.

Review Reference:

Documentation: DeMier, W.V., M.O. Cloninger, H.C. Burkholder, and P.J. Liddell. GETOUT -- A Computer Program for Predicting Radionuclide Decay Chain Transport Through Geologic Media. PNL-2970, Pacific Northwest Laboratory, Richland, Washington, August 1979.

HCTM

Model Type: Unsaturated Ground Water Flow/ Solute Transport

Author: INTERA Technologies Inc.
11999 Katy Freeway, Suite 610
Houston, Texas 77079

Sponsoring Agency: Unknown

Description: HCTM (Hydrology Contaminant Transport Model) is a three-dimensional model that solves both the ground water flow and solute transport equations. The ground water flow equation is solved using a finite difference technique while the trace contaminant equation can be solved by either finite differences or a particle tracking (MOC) scheme. Dispersion and decay are considered as well as linear or non-linear adsorption isotherms or reaction kinetics. However generation is not considered.

Review Reference: SAI, CEC, documentation below

Documentation: Intera Environmental Consultants, Hydrology Contaminant Transport Model: Theory, Implementation and User Input, February 1982.

HYDRO

Model Type:	Unsaturated Ground Water Flow/ Solute Transport
Author:	B. Amirijafari Science Applications, Inc. 1546 Cole Boulevard Golden, CO 80401
Sponsoring Agency:	EG&G Idaho
Description:	HYDRO is a one-dimensional finite difference model capable of simulating unsaturated ground water flow and the transport of up to 20 radioactive nuclides. Soil properties can vary spatially (as a function of grid blocks) and both radioactive decay and adsorption are considered.
Review Reference:	SAI
Documentation:	Amirijafari, B., and B. Cheney, 1979. Simulation of Radionuclide Transport in the Unsaturated Zone Beneath the Radioactive Waste Management Complex, Report submitted to EG&G, June.

ISOQUAD2/PINDER

Model Type: Solute Transport

Author:

George Pinder
Princeton University
Princeton, NJ 08540

Emil Frind
University of Waterloo
Waterloo, Ontario

Sponsoring Agency: Unknown

Description: This model solves the trace contaminant transport equation using a Galerkin finite element method with various possible basis functions. The model is limited to two-dimensional aquifer systems but can be used for both steady and unsteady flow systems.

Review Reference: EPRI, SAI, CEC

Documentation: Pinder, G.F., 1973. A Galerkin-Finite-Element Simulation of Groundwater Contamination on Long Island, New York, Water Resources Research, Vol. 9, No. 6, pp. 1657-1669.

GTC

KONBRED/U.S.G.S.M.O.C

Model Type: Saturated Ground Water Flow, Solute Transport

Author:
L.F. Konikow and J.D. Bredehoeft
U.S. Geological Survey
National Center, Mail Stop 413
Reston, Va 22092

Sponsoring Agency: USGS

Description: The model solves both the ground water flow and solute transport equations. The model uses a finite difference approximation to solve the ground water flow equation and the method of characteristics to solve the solute transport equation and a two step explicit procedure to solve a finite difference equation to describe the effects of hydrodynamic dispersion, fluid sources/sinks and divergence of velocity. The solute is assumed non-reactive while the aquifer fluid is isothermal with constant density. The model may be applied to two-dimensional anisotropic and heterogeneous systems.

Review Reference: EPRI, SAI, CEC, SCEPTER, NRC

Documentation: Konikow, L.F. and J.D Bredehoeft, 1978. Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water, Chapter C2, in Book 7, Techniques of Water Resources Investigations of the USGS.

NRC LPGS

Model Type: Solute Transport/Saturated Ground Water Flow

Author: R.B. Codell
U.S Nuclear Regulatory Commission
Washington, D.C. 20555

Sponsoring Agency: USNRC

Description: Two main models comprise NRC's collection of ground water computer programs. The first program, GROUND, can be used to calculate the concentration and flux from a variety of sources for a single radioactive component. This model is three dimensional and subject to the following assumptions: constant aquifer thickness, constant flow velocity, equilibrium adsorption and a horizontal line source. The second program GRDFLX is similar to GROUND although many more radionuclides can be considered. Both of these models use semi-analytical solutions to the transport equations. NRC also uses a number of analytical solutions to obtain point concentrations and mass fluxes for various source configurations.

Review Reference: Documentation below

Documentation: Codell R.B., K.T. Key and G. Whealen. A Collection of Mathematical Models for Dispersion in Surface Water and Ground Water NUREG 0868, U.S. Nuclear Regulatory Commission, Liquid Pathway Generic Study NUREG-0440, February, 1978.

NWFT/DVM

Model Type:	Solute Transport
Author:	J.E. Campbell INTERA Technologies Inc. 11999 Katy Freeway, Suite 610 Houston, Texas 77079
Sponsoring Agency:	USNRC
Description:	NWFT/DVM (Network Flow and Transport/Distributed Velocity Method) simulates a scenario velocity field as a network of one-dimensional segments through which radionuclides are transported. The DVM method allows for the transport of decay chains of any length, with isotopes having different retardations and source rates being leach or solubility limited.
Review Reference:	NRC, CEC, SAI, SCEPTER
Documentation:	Campbell J.E., D.E. Longsine, and R.M. Cranwell, 1981. Risk Methodology for Geologic Disposal of Radioactive Waste: The NWFT/DVM Computer Code Users Manual, NUREG/CR2081. Sand 81-0886, November 1981.

OGRE

Model Type: Saturated Ground Water Flow and Solute Transport

Author: J.A. Korver
Lawrence Livermore Laboratory
Livermore, CA 94550

Sponsoring Agency: USDOE

Description: OGRE simulates fluid flow and mass transport through heated porous medium. The model is applicable to one or two-dimensional systems and is fully transient (both flow and solute).

Review Reference: EPRI, CEC, SAI

Documentation: Korver, J.A., 1970. UCRL-50820, Lawrence Livermore Laboratory, Livermore, CA, February.

PATHS

Model Type:	Saturated Ground Water Flow and Solute Transport
Author:	R. William Nelson Manager, Nuclear Waste Materials Characterization Center Battelle Pacific Northwest Laboratories P.O. Box 999 Richland, WA 99352
Sponsoring Agency:	USDOE
Description:	PATHS uses analytical solutions for the ground water potential distribution to construct differential equations of fluid particle pathlines. These equations are solved numerically to given particle positions as a function of time. The model can be used for two dimensional, saturated steady or transient flow systems. Geochemical retardation is considered but dispersion is ignored.
Review Reference:	SAI, NRC, EPRI, CEC
Documentation:	Nelson, R.W. and J.A. Schur, 1980. PATHS - Ground Water Hydrologic Model (Assessment of Effectiveness of Geologic Isolation Systems), PNL-3162, Pacific Northwest Laboratory, Richland, WA, April.

PCP

Model Type:	Solute Transport Model
Author:	D.R. Friedrichs, C.R. Cole, and R.C. Arnett Atlantic Richfield Hanford Company Richland, WA 99352
Sponsoring Agency:	ERDA
Description:	PCP (Path-line Calculational Program) can be used to determine two-dimensional path-lines for specified ground water flow regimes. The model uses a semi-analytical technique.
Review Reference:	SAI
Documentation:	Friedrichs, D.R., C.R. Cole and R.C. Arnett, 1977. Hanford Pathline Calculational Program - Theory, Error Analysis and Applications, ARH-ST-149, Atlantic Richfield Hanford Company, Richland, WA, June. ARH-ST-149.

PERCOL

Model Type: Solute Transport

Author: R.C. Routson
Argonne National Laboratory
Energy and Environmental Systems Division
9700 S. Cass Avenue
Argonne, IL 60439
FTS 972-3416

R.J. Serne
Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USGS

Description: PERCOL is a one-dimensional model of radionuclide transport through porous media. The model considers sorption, ion exchange hydrodynamic dispersion and diffusion. The model can include the effect of partial saturation although a constant flow rate is assumed.

Review Reference: SAI

Documentation: Routson, R.C. and R.J. Serne, 1972. One-Dimensional Model of the Movement of Trace Radioactive Solute Through Soil Columns: The PERCOL Model, BNWL-1718, Battelle Pacific Northwest Laboratories, Richland, WA.

ROBERTSON 2/INEL TRANSPORT I

Model Type: Saturated Ground Water and Flow and Solute Transport

Author:
J.B. Robertson
U.S. Geological Survey, National Center
12201 Sunrise Valley Drive
Reston, VA 22092
(703) 860-6976

Sponsoring Agency: USGS

Description: ROBERTSON 2 consists of two coupled subprograms: one calculates ground water velocities in a two-dimensional single layer aquifer, the second simulates solute transport through the system. The ground water flow velocities are calculated as functions of space and time using a finite difference technique. The transient solute transport equation is solved using a method of characteristics approach. Processes considered in the solute transport portion include radioactive decay, dispersion, convection, adsorption and ion exchange. The model has successfully simulated radionuclide plume movement in ground water.

Review Reference: SAI, CEC

Documentation: Robertson, J.B., 1974. U.S. Geological Survey, National Reactor Testing Station, Idaho Falls, ID.

SALTRP

Model Type:	Saturated Ground Water and Flow and Solute Transport
Author:	L. Picking Stone and Webster Engineering P.O. Box 2325 Boston, MA 02107
Sponsoring Agency:	USDOE
Description:	SALTRP is a two-dimensional model for simulating the dissolution of and transport through the ground water of a salt bed. The model uses a Galerkin finite element technique to solve the fluid and salt continuity equations for the finite element grid.
Review Reference:	SAI
Documentation:	Unavailable

GTC

SEGOL

Model Type: Saturated/Unsaturated Ground Water Flow and Solute Transport

Author:
G.A. Segol
Bechtel
P.O. Box 3965
San Francisco, CA 94119

Sponsoring Agency: Unknown

Description: SEGOL is a three-dimensional model capable of simulating flow and solute transport through saturated/unsaturated media. The transport equations are solved using a Galerkin finite element method with either linear, quadratic or cubic isoparametric quadrilateral elements. Both flow and solute transport may be transient.

Review Reference: SAI, EPRI, CEC

Documentation: Segol, G.A., 1976. A Three-Dimensional Galerkin Finite Element Model for the Analysis of Contaminant Transport in Variably Saturated Porous Media -- User's Guide, Department of Earth Sciences, University of Waterloo, Waterloo, Ontario.

STM

Model Type: Ground Water Flow and Solute Transport

Author:
D.B. Grove
U.S. Geological Survey
Denver Federal Center
Denver, CO 80225

J. Rubin
U.S. Geological Survey
345 Middlefield Road
Menlo Park, CA 94025

Sponsoring Agency: USGS

Description: STM (Solute Transport Model) is comprised of two submodels; one calculates ground water flow velocities while the second uses those velocities in its transport calculations. The solute transport model considers such processes as convection; hydrodynamic dispersion, ion exchange rates, rate-controlled chemical reactions and radioactive decay. Both one and two dimensional systems can be analyzed.

Review Reference: SAI, CEC

Documentation: Grove, D.B., and J. Rubin, 1976. Disposal of Residues on Land, CONFE-760968, Proceedings of a National conference held in St. Louis, Missouri, September 13-15, 1976, U.S. Geological Survey, Denver, CO and Menlo Park, CA, pp. 174-178.

SWIFT

Model Type: Solute Transport Saturated Ground Water Flow

Author: INTERA Technologies Inc.
11999 Katy Freeway, Suite 610
Houston, Texas 77079

Sponsoring Agency: USNRC

Description: SWIFT (Sandia Waste Isolation Flow and Transport Model) is a three-dimensional model capable of simulating ground-water flow, trace radionuclide chain transport, brine (density dependent) transport and heat transport in porous media. The model can solve all or any combination of the equations representing these processes using a finite difference approach. Fluid density can be a function of pressure, temperature and concentration while viscosity can be a function of temperature and concentration. Several sub-models of the model allow for the simulation of a nuclear waste repository including such processes as leaching, dissolution and decay/generation of the nuclide inventory. The model also possesses a sophisticated well-bore sub-model.

Review Reference: SAI, EPRI, CEC, Documentation below

Documentation: Reeves, M. and R.M. Cranwell, 1981. User's Manual for the Sandia Waste Isolation Flow and Transport Model (SWIFT), Release 4.81, SAND 81-2516, NUREG/CR-2324, Sandia National Laboratories, Albuquerque, N.M.

Reeves, M., N.D. Johns and R.M. Cranwell. Input Data Guide for SWIFT II. The Sandia Waste Isolation Flow and Transport Model for Fractured Media, to be published as a SAND-NUREG report, Sandia National Laboratories, Albuquerque, N.M.

SWIP

Model Type:	Solute Transport (Saturated Ground Water Flow)
Author:	INTERA Technologies Inc. 11999 Katy Freeway, Suite 610 Houston, Texas 77079
Sponsoring Agency:	USGS
Description:	SWIP is a transient three-dimensional subsurface waste disposal model which solves the pressure, energy and mass-transport equations using a finite difference method. Viscosity and density are dependent upon temperature and concentration. The model can be used for one, two or three dimensional cartesian or radial systems. The model possesses a sophisticated well-bore sub-model which can simulate pressure drop through a tubing string and heat loss from the well-bore.
Review Reference:	EPRI, documentation below
Documentation:	INTERA Environmental Consultants, Inc., 1976. A Model for Calculating Effects of Liquid Waste Disposal in Deep Saline Aquifer, Part I- Development, Part II - Documentation. Houston, Texas, June 1976.

TRANSAT

Model Type: Solute Transport Saturated Ground Water Flow

Author: J.F. Pickens
GTC Geologic Testing Consultants
Ottawa, Ontario K1S 5H4

Sponsoring Agency: none

Description: TRANSAT simulates two-dimensional solute transport in a saturated steady-state flow field. The trace contaminant is subject to decay, reversible sorption and dispersion. A Galerkin finite element technique is used to solve both flow and transport equations.

Review Reference: CEC, EPRI, WISAP

Documentation: Grisak, G.E., J.F. Pickens, J.A. Cherry, 1980. Solute Transport Through Fractured Media - 2. Column Study of Fractured Till, Water Resources Research, Vol. 16, No. 4, pp. 731-739.

Pickens, J.F., and G.E. Grisak, 1981. Scale-Dependent Dispersion in a Stratified Granular Aquifer, Water Resources Research, Vol. 17, No. 4, pp. 1191-1211.

Pickens, J.F., and G.E. Grisak, 1981. Modeling of Scale Dependent Dispersion in Hydrogeologic Systems. Water Resources Research, Vol. 17, No. 6, pp.1701-1711.

TRENCH

Model Type:	Solute Transport
Author:	Oktay Oztunoli Dames & Moore 20 Harlem Avenue White Plains, NY 10603
Sponsoring Agency:	AIF
Description:	TRENCH simulates the migration of radionuclides from a burial trench relating the quantity leaving the trench to that crossing a hypothetical boundary. The medium is assumed homogeneous and isotropic, the fluid incompressible with a constant viscosity. Transport processes which are considered include dispersion (lateral and longitudinal), convection, reversible ion exchange and radioactive decay (but no generation). The model does not perform ground water flow calculations and hence requires a velocity field as input.
Review Reference:	CEC, SAI
Documentation:	Generic Methodology for Assessment of Radiation Doses from Groundwater Migration of Radionuclides in LWR Wastes in Shallow Land Burial Trenches, 1979, AIF/NESP-013, American Information Forum, January.

UCB-NE-10, UCB-NE-30

Model Type: Solute Transport Models

Author: F. Iwamoto and A. Fujita
Department of Nuclear Engineering
University of California
Berkeley, CA 94720

Sponsoring Agency: USDOE

Description: UCB-NE-10, UCB-NE-30 are two computer programs developed to analyze the one-dimensional migration of a radionuclide chain through porous media. UCB-NE-30 differs from UCB-NE-10 in that it can handle up to 6 member decay chains, lateral dispersion, and up to two media. Release mechanisms differ between the codes, UCB-NE-10 uses banded, impulse or exponential release rates while UCB-NE-30 can be banded, linear or quadratic. The codes are based on analytical solutions of Harada et al. (1980) and Pigford et al. (1980).

Review Reference: Documentation below

Documentation: Harada, M., P.L. Chambré, M. Foglia, K. Higashi, F. Iwamoto, D. Leung, T.H. Pigford and D. Ting, 1980. Migration of Radionuclides Through Sorbing Media: Analytical Solutions - I, LBL-10500, UC-71.

T.H. Pigford, P.L. Chambré, M. Albert, M. Foglia, M. Harada, F. Iwamoto, T. Kanki, D. Leung, S. Masuda, S. Muraoka and D. Ting, 1980. Migration of Radionuclides Through Sorbing Media Analytical Solution II, LBL-11616, UC-70.

SURFACE WATER

TRANSPORT MODELS

Table 4. Capabilities of Surface Water Models

Model	Water Body[1]	Dimensionality	Time Dependence	Solution Technique[2]	Sediment	Rad. Decay	Comments
CHMSED	R	1	S.S.	FD	Y	N	
DPRW	L,O	2,3	T	DRRW*	N	N	*Discrete parcel random walk
FETRA	E,O,R	2	S.S.	FE	Y	Y	Field application
HERMES-WTRAN	R,L	1	T	FD	Y	Y	
HOTSED	E,R	1	T	I	Y	N	Does not consider dissolved radionuclides
NRC-LPGS	R,L,E	1	S.S., T	A	Y	Y	Field applications
SEDTRN	R	1	S.S.	FD	Y	N	No contaminant transport
SEDONE	R,E	1	T	FD	Y	N	
SERATRA/ TODAM	R,L	2	T	FE	Y	Y	
TEHM/UTM	R,W	1	T	A, FD	N	N	Watershed model No transport
White & Gloyna	R	1	T	FD	Y	N	
WHTM/UTM	R,W	1	T	A, FD	Y		Based on Standford Watershed model

[1] R = rivers, L = lakes, O = oceans, E = estuaries, W = watershed

[2] FD = finite difference, FE = finite element, A = analytical, I = integration

CHNSED

Model Type: Surface Water Transport

Author:
D.E. Fields
Nuclear Division
Union Carbide Corporation
P.O. Box X
Oak Ridge, TN 37830

Sponsoring Agency: NSF Ecology and Trace Analysis Program

Description: CHNSED is comprised of two sub-models, SEDTRN and WHTM. SEDTRN simulates the transport of sediment through a rectangular stream channel system, while WHTM is a processes model. Processes considered in CHNSED include sheet erosion, overland tranport, and dissolved contaminant transport. An ion exchange sub-model simulates the soil-contaminant water interaction at the land surface and partitioning between sediment and water in the channel. Adsorbed contaminant movement is controlled by sediment transport dynamics which are categorized as either bedload or suspended load. Mannings equation is used to determine flow rate while Stokes Law is used to describe particle deposition.

Review Reference: SAI, SCEPTER

Documentation:

Fields, D.E., 1976a. LINSED: A One Dimensional Multireach Sediment Transport Model, ORNL/CSD-15, Oak Ridge National Laboratory, Oak Ridge, TN, October.

Fields, D.E., 1976b. Simulation of Sediment and Trace Contaminant Transport with Sediment-Contaminant Interaction, ORNL/NSF/EATC-10, Oak Ridge National Laboratory, Oak Ridge, TN, March.

Fields, D.E. and D.M. Hetrick. HOTSED: A Discrete Element for Simulating Hydrodynamic Conditions and Adsorbed and Dissolved Radioisotope Concentrations in Estuaries, NUREG/TM-266, U.S. Nuclear Regulatory Commission (in press).

Patterson, M.R., J.K. Munro, D.E. Fields, R.D. Ellison, A.A. Brooks, and D.D. Huff, 1984. A User's Manual for the FORTRAN IV Version of the Wisconsin Hydrologic Transport Model, ORNL/NSF/EATC-7, Oak Ridge National Laboratory, Oak Ridge, TN, October.

FETRA

Model Type: Surface Water Transport

Author: Y. Onishi, P.A. Johanson, F.G. Baca, and E.I. Hilty
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: Unknown

Description: FETRA is a two-dimensional (planar) finite element model for sediment-contaminant transport applicable to wide, shallow water bodies. The model considers transport of both dissolved and adsorbed radionuclides.

Review Reference: SAI, SCEPTER, NRC(2)

Documentation: Onishi, Y., E.M. Arnold and D.W. Mayer. 1979. Modified Finite Element Transport Model, FETRA, for Sediment and Radionuclide Migration in Open Coastal Waters. NUREG/CR-1026. PRN1-3114, Pacific Northwest Laboratory, Richland, WA.

HOTSED

Model Type: Surface Water Transport

Author: D.E. Fields and D.M. Hetrick
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: HOTSED was developed to simulate the movement of radionuclides both dissolved and adsorbed onto sediment through estuaries. The model resulted from combining the sediment transport model SEDTRN to a one-dimensional model for simulating hydrodynamic, thermal and dissolved radionuclide concentrations in estuaries. The model has been used to simulate radioisotope bearing sediment in the Hudson River under transient tidal conditions.

Review Reference: SAI

Documentation: N/A

NRC-LPGS

Model Type: Surface Water Transport

Author: U.S. Nuclear Regulatory Commission

Sponsoring Agency: Unknown

Description: USNRC has been undertaking a Liquid Pathways Generic Study and has developed a number of simple analytical models to describe radionuclide transport in various surface water bodies. Three models describing the radionuclide transport and sediment interactions comprise the package. All three models consider radioactive decay and have been applied to various field sites. The estuary and river models are one-dimensional while the lake model is assumed to be comprised of a number of completely mixed regions.

Review Reference: SCEPTER, NRC(2)

Documentation: U.S. Nuclear Regulatory Commission, 1978a. Liquid Pathway Generic Study. Impacts of Accidental Radioactivity Releases to the Hydrosphere from Floating and Land-Based Nuclear Power Plants. NUREG-0440.

SEDONE

Model Type: Surface Water Transport

Author: D.M. Hetrick, A.H. Eraslan, and M.R. Patterson
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: SEDONE was developed to simulate hydrodynamic conditions and sediment concentrations in estuaries and controlled rivers. The model is one-dimensional and considers settling and resuspension of sediment. No radionuclide transport is considered.

Review Reference: SAI, SCEPTER

Documentation: Hetrick, D.M. A.H. Eraslan, and M.R. Patterson, 1984. ORNL/NUREG/TM-256, Oak Ridge National Laboratory, Oak Ridge, TN, November, p.285.

SEDTRN

Model Type: Surface Water Transport

Author: Unknown

Sponsoring Agency: Unknown

Description: SEDTRN simulates steady-state sediment transport in a uniform rectangular open channel. The model considers such mechanisms as sheet erosion and overland flow. Sediment within the channel is characterized as either resident, suspended or bedload sediment. The model does not consider trace contaminant transport.

Review Reference: SCEPTER

Documentation: Unknown

SERATRA/TODAM

Model Type: Surface Water Transport

Author: Y. Onishi, P.A. Johanson, F.G. Baca, and E.I. Hilty
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: Unknown

Description: SERATRA (SEdiment RAdionuclide TRAnsport) is a transient two-dimensional model capable of describing radionuclide migration in rivers and estuaries. SERATRA solves the general advection diffusion equation using a finite-element method. The model considers radionuclide decay and transport of both dissolved and adsorbed radionuclides. The model assumes uniform mixing across the river. SERATRA has been simplified to a one-dimensional longitudinal model TODAM (Transient One-Dimensional Degradation and Migration)

Review Reference: SAI, SCEPTER, NRC(2)

Documentation: Onishi, Y. and S.E. Wise, 1979b. Mathematical Model, SERATRA, for Sediment-Contaminant Transport in Rivers and Its Application to Pesticide Transport in Four Mile and Wolf Creeks in Iowa. Submitted to U.S. Environmental Protection Agency, Environmental Research Laboratory at Athens, GA. by Battelle Pacific Northwest Laboratories, Richland, WA.

TEHM

Model Type: Surface Water Transport

Author: D.Huff, R. Luximoore, J. Mankin and C. Begovich
Environmental Sciences Division
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: Unknown

Description: TEHM (Terrestrial Ecosystem Hydrology Model) simulates interception, infiltration, evaporation, transpiration, saturated and unsaturated ground water flow, surface run-off and open channel flow. Most of the processes are described by mechanistic models. The model does not consider nuclide transport.

Review Reference: SAI, SCEPTER

Documentation: TEHM: A Terrestrial Ecosystem Hydrology Model, ORNL/NSF/EATC-27, Oak Ridge National Laboratory, Oak Ridge, TN, pp. V.I., 74.

UTM

Model Type: Surface Water Transport

Author: M.R. Patterson (ORNL)
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: Unknown

Description: UTM (Unified Transport Model) simulates the transport, accumulation and redistribution of trace contaminants in air, and surface water bodies. This model is comprised of several submodels each of which is a stand alone model, for example, CHNSED, CHANL, WHTM, etc. The surface water portion of the model considers the transport of dissolved and suspended materials in stream channel. Sediment transport and mixing and exchange between aqueous and solid phases is simulated.

Review Reference: SAI, SCEPTER

Documentation: VanHook, R.I. and W.D. Shults, Editors. Ecology and Analysis of Trace Contaminants Progress Report (Oct. 74-Dec.75), ORNL/NSF/EATC-22, Oak Ridge National Laboratory, Oak Ridge, TN.

WHITE AND GLOYNA

Model Type: Surface Water Transport

Author: A. White and E.F. Gloyna
University of Texas
Austin, Texas

Sponsoring Agency: Unknown

Description: The White and Gloyna (1969) model is capable of simulating transient one-dimensional radionuclide transport by accounting for radionuclide adsorption/desorption with bed sediment and aquatic plants. The model does not consider transport, deposition or resuspension of sediment. This model is similar to other models developed by Gloyna and his associates including Armstrong and Gloyna (1968) and Shih and Gloyna (1967).

Review Reference: SCEPTER, NRC(2)

Documentation: White, A. and E.F. Gloyna, 1969. Radioactivity Transport in Water -- Mathematical Simulation. EHE-70-04, Technical Report No. 19 to the U.S. Atomic Energy Commission, University of Texas, Austin, TX.

Armstrong, N.E. and E.F. Gloyna, 1968. Numerical Solutions of Radionuclide Transport, Chemical Engineering Progress Symposium Series. 64(90):47-58.

Shih, C.S. and E.F. Gloyna, 1967. Radioactivity Transport in Water -- Mathematical Model for the Transport of Radionuclides. EHE-04-6702, Technical Report No. 12 to the U.S. Atomic Energy Commission, University of Texas, Austin, TX.

WHTM

Model Type:	Surface Water Transport
Author:	R.Raridon, J. Munro, Jr., M. Patterson, and D. Fields Computer Sciences Division Union Carbide Corporation, Nuclear Division Oak Ridge, TN 37830
Sponsoring Agency:	Unknown
Description:	WHTM (Wisconsin Hydrologic Transport Model) is a component of UTM (Unified Transport Model) and simulates the movement of water and trace contaminants from the time they are deposited on the land surface, down through the soil to the water table or across the land surface to the surface water network and eventually the watershed outfall. Chemical exchange is simulated using an ion-exchange submodel together with a sheet erosion submodel. Most of the submodels use a lumped parameter description of the transport processes.
Review Reference:	SAI
Documentation:	1974. A User's Manual for the FORTRAN IV Version of the Wisconsin Hydrologic Transport Model, ORNL-NSF-EATC-7 (EDFB-1BP-74-9).

WTRAN

Model Type: Surface Water Transport

Author: J.F. Fletcher and W.L. Dotson
Hanford Engineering Development Laboratory
Richland, WA 99352

Sponsoring Agency: USDOE

Description: WTRAN is a HERMES submodel designed to calculate concentrations of both dissolved and adsorbed radionuclides. It is one-dimensional, consisting essentially of a number of connected completely mixed cells. Sources/sinks from each of the cells can be used to simulate various processes such as overbank deposition, atmospheric contribution, etc. Both steady-state and transient calculations can be performed. Other processes considered include first-order decay and adsorption.

Review Reference: SAI, SCEPTER, documentation below

Documentation: Fletcher, J.F. and W.L. Dotson, 1971. HERMES: A Digital Computer Code for Estimating Regional Radiological Effects from the Nuclear Power Industry, HEDL-TME-71-168, Hanford Engineering Development Laboratory, Richland, WA, 759 pp.

Soldat, J.K., 1971. Modeling of Environmental Pathways and Radiation Doses from Nuclear Facilities, USAEC Report BNWL-SA-3939, Battelle Pacific Northwest Laboratories, October.

DOSE FROM LIQUID PATHWAYS

MODELS

Table 5. Capabilities of Dose Through Liquid Pathways Models

Model	Surface Water Transport		Dose Calculations			Comments
	Type	Sedimentation	Ingestion Aquatic/Terrestrial Food	Immersion/ Exposure	Ind./Population	
AQUAMAN			A	Y	I	
AQUAMOD	Compartment Model	Compartment Model	N	N		Gives equilibrium conc. in sed. & water
ARRRG	Compartment Model	N	A	Y	I,P	HERMES submodel
BIODOSE	Compartment Model	Compartment Model	A,T	Y	I	Requires transfer coefficients NUTRAN member
CARDOCC	N	N	A			This model interfaces with ARRRG
CUEX			A			
FOOD	Compartment Model	N	T	N		HERMES submodel
LADTAP II	Compartment Model	N	A,T	Y	I,P	Considers infants, children, teenagers & adults
PABLM	Compartment Model	- uses Kd - assumes equilibrium	A,T	Y	I,P	Adults only; organs & body
PATH1	Compartment Model	- uses Kd - assumes equilibrium	A,T*			-Requires Transfer coefficients -*Concentration not dose
PLUTRAN				Y	I	Considers ^{239}Pu only
RVRDOS	Rivers		A	Y	I,P**	-**population dose for ingestion -individual dose for immersion

AQUAMAN

Model Type: Dose from Liquid Pathways

Author/Contact: D.L. Shaeffer and E.L. Etnier

Sponsoring Agency: Unknown

Description: AQUAMAN calculates the 50 year dose commitment to man resulting from the release of radionuclides to the aquatic environment. The model uses its own data base to provide dose conversion and bioaccummulation facts (for both freshwater and marine environments). Dose for total body, GI tract, bone, thyroid, lungs, liver, kidneys, and gonads can be calculated for three potential pathways - water ingestion, fish ingestion and immersion.

Review Reference: SAI

Documentation: Pfuderer, H. and C. Johnson. Data Search Performed on Energy Data Base, Oak Ridge National Laboratory, Oak Ridge, TN.

AQUAMOD

Model Type: Dose from Liquid Pathways

Author:
R.S. Booth
P.O. Box X
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: AQUAMOD was designed principally to simulate radionuclide interaction between water and sediment. This is achieved through a four compartment model representing the receiving water, water and bottom sediments, sediment subject to sorption/desorption and sediment subject to only sorption mechanisms. Sediment concentrations can be used to calculate external dose.

Review Reference: SAI, SCEPTER, NS

Documentation: Booth, R.S., 1975. "Systems Analysis Model for Calculating Radionuclide Transport Between Receiving Waters and Bottom Sediments", Environmental Toxicity of Aquatic Radionuclides: Models and Mechanisms, USAEC Report ORNL/TM-4751, Oak Ridge National Laboratory, Oak Ridge, TN, April.

ARRRG

Model Type:	Dose from Liquid Pathways
Author:	J.K. Soldat, N.M. Robinson and D.A. Baker Battelle Pacific Northwest Laboratories Box 999 Richland WA, 99352
Sponsoring Agency:	USDOE
Description:	ARRRG (Aqueous Reactor Release Result Generator) can be used to calculate annual individual and population doses resulting from radionuclide releases in liquid effluents. The model can calculate the dose to skin, whole body, GI tract, thyrod, bone, liver, lungs and kidneys via ingestion, immersion or exposure pathways. The program requires the input of reconcentration factors and mixing ratios.
Review Reference:	SAI, SCEPTER, NS
Documentation:	Nepier, B.A., et al., 1980. ARRRG and FOOD - Computer Programs for Calculating Radiation Dose to Man from Radionuclides in the Environment, DE-AC06-76RLO-1830, Battelle Pacific Northwest Laboratories, Richland, WA, June. Shriner, C.R. and L.J. Peck, 1978. Inventory of Data Bases, Graphics Packages, and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November. Soldat, J.K., N.M. Robinson, and D.A. Baker, 1974. Models and Computer Codes for Evaluating Environmental Radiation Doses, BNWL-1754, Battelle Pacific Northwest Laboratories, Richland, WA.

BIODOSE

Model Type: Dose from Liquid Pathways

Author: J.J. Duffy and G.P. Bogar
The Analytic Sciences Corporation
One Jacob Way
Reading, MA 01867

Sponsoring Agency: USNRC

Description: BIODOSE is a member of the NUTRAN systems model and calculates the biosphere transport and dose to man resulting from radionuclide release from a high level nuclear waste disposal site. Processes affecting radionuclide transport are modeled as compartments with transfer coefficients describing the coupling between different compartments. Dilution, diffusion between sediment and water, sedimentation, removal of water and food by man, ion exchange, biogeochemical processes and radioactive decay are all considered. Dose by ingestion and exposure are both considered.

Review Reference: SAI, SCEPTER, NRC(3)

Documentation: Berman, L.E., D.A. Ensminger, M.S. Guiffre, C.M. Koplik, S.G. Oston, G.D. Pollak, and B.I. Ross, 1978. Analysis of Some Nuclear Waste Management Options, UCRL-13917, The Analytic Sciences Corporation, Reading, MA, December.

Bonner, N.A., et al, 1979. Preliminary Evaluation of the BIODOSE Computer Program, UCID-18267, University of California, Livermore, CA, September.

Duffy, J.J., and G.P. Bogar, 1980. User's Manual for Biosphere and Dose Simulation Program (BIODOSE), Lawrence Livermore Laboratory, Livermore, CA.

CARDOCC

Model Type:	Dose from Liquid Pathways
Author:	J.R. Watts Savannah River Laboratory Aiken, SC 29801
Sponsoring Agency:	USDOE
Description:	CARDOCC calculates 70 year dose commitments resulting from chronic ingestion through aqueous pathways. Dose is calculated for whole body, bone, LLI and six internal organs.
Review Reference:	SAI
Documentation:	Watts, J.R. 1976. Modeling of Radiation Doses from Chronic Aqueous Releases, ERDA Report CONF-760652-1, Savannah River Laboratory, Aiken, SC.

FOOD

Model Type: Dose from Liquid Pathways

Author: D.H. Denham, D.A. Baker, J.K. Soldat and J.P. Corley
Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: FOOD is part of the HERMES systems model and calculates annual individual doses and population due to the ingestion of food contaminated from air deposition or water (irrigation). The model requires the input of such parameters as irrigation rates, air concentration, mixing ratios, reconcentrations factors, etc.

Review Reference: SAI, SCEPTER, NS

Documentation: Baker, D.A., G.R. Hoernes, and J.K. Soldat, 1976. FOOD: An Interactive Code to Calculate Internal Radiation Doses from Contaminated Food Products, ERDA Report BNWL-SA-5523, Battelle Pacific Northwest Laboratoires, Richland, WA.

Denham, D.H., D.A. Baker, J.K. Soldat, and J.P. Corley, 1973. Radiological Evaluations for Advanced Waste Management Studies, BNWL-1764, Battelle Pacific Northwest Laboratories, Richland, WA.

LADTAP II

Model Type: Dose from Liquid Pathways

Author: D.B. Simpson and B.L. McGill
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USNRC

Description: LADTAP II calculates the dose to man from pathways in the aquatic environment in accordance with USNRC Regulatory Guide 1.109. Doses are calculated for both the maximally exposed individual and general population for various organs, age groups and pathways. A companion library provides dose factors for various age groups and organs. The dose pathways include ingestion, immersion and exposure. Dispersion in the aquatic environment can be modeled assuming no reconcentration, complete or partial mixing or plug flow.

Review Reference: SAI, SCEPTER, NRC(3)

Documentation: Simpson, D.B. and B.L. McGill, 1980. User's Manual for LADTAP II - Computer Program for Calculating Radiation Exposure to Man from Routine Release of Nuclear Reactor Liquid Effluents. NUREG/CR-1276. ORNL/NUREG/TDMC-1.

PABLM

Model Type: Dose from Liquid Pathways

Author: B.A. Napier, W.E. Kennedy, Jr. and J.K. Soldat
Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: PABLM can be used to calculate the dose to man resulting from radionuclide release to stream water or the use of contaminated irrigation water. The model can also be used to calculate the dose to man from atmospheric concentrations of radionuclides. The majority of the data required by the code (e.g., dose factors, radionuclide parameter) are contained in companion libraries. The code considers ingestion and exposure pathways.

Review Reference: SAI, SCEPTER

Documentation: Napier, B.A., W.E. Kennedy, Jr., et al., 1980. PABLM - A Computer Program to Calculate Accumulated Radiation Doses from Radionuclides in the Environment, PNL-3209. Pacific Northwest Laboratory, Richland, WA,

PATH1

Model Type: Dose from Liquid Pathways

Author: Jon Helton
Sandia Laboratories
Albuquerque, NM 87185

Sponsoring Agency: USNRC

Description: PATH1 simulates the transport of radionuclides to man via various pathways and calculates the resulting dose. PATH1 is divided into several submodels including the Environmental Transport Model, Transport to Man Model and the Dosimetry Model. The Environmental Transport Model uses a four-compartment model in which each compartment has a transporting medium (water) and an adsorbing medium (soil). Each compartment is assumed to be completely mixed with transport between compartments. Nuclide decay and generation is considered. Ingestion and inhalation of radionuclides is determined by the Transport to Man Model. The final dose calculated by the Dosimetry Model includes the effects of ingestion, inhalation and immersion.

Review Reference: SAI, NRC(3), SCEPTER

Documentation: Campbell, J.E., et al, 1978. Risk Methodology for Geologic Disposal of Radioactive Waste: Interim Report, SAND78-0079, Sandia National Laboratories, NUREG/CR-0458, prepared for the U.S. Nuclear Regulatory Commission, October.

Helton, J.C., and P.C. Kaestner, 1981. Risk Methodology for Geologic Disposal of Radioactive Waste: Model Description and User's Manual, the Pathways Model. NUREG/CR-1636, Vol. 1. SAND 78-1711 AN.

RVRDOS

Model Type: Dose from Liquid Pathways

Author: J. Martin, Jr., C. Robbins, C. Nelson, R. Cousins and M. Culliton

Sponsoring Agency: Unknown

Description: RVRDOS calculates the dose to the population resulting from the release of radionuclides in streams. Processes such as dilution, decay, and generation are considered. Population doses to four organs from the ingestion pathway and individual immersion doses may be calculated.

Review Reference: SAI

Documentation: Martin, J.A., Jr., C. Robbins, C.B. Nelson, R.D Cousins, Jr., M.A. Culliton, 1976. A Computer Code (RVRDOS) to Calculate Population Doses from Radioactive Liquid Effluents and on Application to Nuclear Power Reactors on the Mississippi River Basin. USEPA, Office of Radiation Programs, Environmental Analysis Division.

DOSE FROM
ATMOSPHERIC PATHWAYS

Table 6. Capabilities of Atmospheric/Dose to Man (Inhalation//Exposure) Models

Model	Atmospheric Transport Processes				Dose Calculations			Comments
	Dispersion	Decay	Suspension	Deposition	Air Exposure	Inhalation	Individual/Population	
ACRA II	Gaussian Plume	Y	N	Y	Y	Y	I	Accidental Release
AIRDOS	Gaussian Plume	Y	N	Y	Y	Y	I,P	Chronic
AIREM	Gaussian Plume	Y	N	Y	Y	Y	I,P	Chronic Release
AIRWAY	Gaussian Plume	Y	Y		Y	Y	I	
AISITE II	Unknown	Y	N	N	Y	Y		Superceded by COMRADEX
AREAC	Gaussian Plume	Y				I	P	
ARTRAN	Gaussian Plume	Y	N	Y				HERMES Submodel
BELCH					Y	Y	I,P	Routine Release
2BPUFF				Y	Y	Y	I,P	Developed for Atmospheric Tests
COMRADEX-IV	Gaussian Plume	Y	N	N	Y	Y	I	Accidental Release
CRAC	Gaussian Plume	Y		Y	N	N		
CUEX, AIRMOD	Unknown				Y			
DACRIN	Gaussian Plume				Y	Y		
EGAD	Gaussian Plume	N	N	N	Y	N	I	
EXDOSE	Gaussian Plume	Y		Y	Y	N	I	
EXGAM	Gaussian Plume	Y			Y	N		

GTC

Table 6 (cont'd)

Model	Atmospheric Transport Processes				Dose Calculations			Comments
	Dispersion	Decay	Suspension	Deposition	Air Exposure	Inhalation	Individual/Population	
EXTREM III	Y	Y	Y		Y	N	I	Accidental Release
FISSP/CLOUD	Gaussian Plume	Y	Y		Y	Y	I	Fission Products only
GADOSE/DOSET	Y	Y		Y	Y	Y		Accidental Release
GAMMA	Gaussian Plume	Y		N	Y	N		Noble Gas Plumes
GAUCHE					Y	Y	I	Calculates annual dose Also ingestion
GRONK	Gaussian Plume			Y	Y	Y		Also ingestion
INDOSE	N	N	N	N	N	Y	I	Organ doses
INGDOSE				Y			I	Calculates ingestion dose due to deposition
INHDOSE	Gaussian Plume	N	Y	Y			I,P	
KRONIC	Plume	Y	Y	N	Y	N	I,P	Chronic Release
MESODIF II	2 D Variable Trajectory			Y	N	N		No dose calculations
NUBE	Plume		N	Y	Y	Y		Gives statistical distribution
PREDO				Y				

Table 6 (cont'd)

Model	Atmospheric Transport Processes				Dose Calculations			Comments
	D'spersion	Decay	Suspension	Deposition	Air Exposure	Inhalation	Individual/Population	
RACER	Gaussian Plume	Y	Y	N	Y	N	I	Accidental Release
RACOS	Gaussian Plume	Y	N	N	Y	N	I	Accidental Release
RSAC-2	Gaussian Plume	Y	N	Y	Y	Y	I	Accidental Release
STAREL/RELISH			N	N	N	N		
SUBCOSA	Y	Y	N	N	Y	N	I	Accidental Release
SUBPOPA	Y	Y	Y		Y	N	P	
THUNDERHEAD	Y		N	N	Y	Y		
UDAD	Gaussian Plume	Y		Y		Y		Used for uranium mine & small operations
VITTLS				Y			I	Food ingestion and ingestion
WRED			N	N	Y	N		Gives prob. dist. on doses
XOQDOQ	Plume			Y	N	N		

ACRA II

Model Type: Dose from Atmospheric Pathways

Author: F.W. Stallman and F.B.K. Kam
Union Carbide Corporation
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: ACRA II was developed for the purpose of calculating inhalation and exposure doses from atmospheric releases of radioactive material during a nuclear reactor accident. The release of radioactive material is assumed to be at a constant rate, while dispersion is assumed to conform to a Gaussian distribution. Radioactive decay is included in the calculation.

Review Reference: SAI, SCEPTER, NS

Documentation: Binford, F.T., J. Barish and F.B.K. Kam, 1968. Estimation of Radiation Doses Following a Reator Accident, ORNL-4086, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN.

Oak Ridge National Laboratory, 1974. RSIC Computer Code Collection: ACRA-II: Kernel Integration Code, Estimation of Radiation Doses Caused by a Hypothetical Reactor Accident, USAEC Report CCC-213, U.S. Atomic Energy Commission, Washington, DC, July.

Stallman, F.W. and F.B.K. Kam, 1973. ACRA - Computer Program for the Estimation of Radiation Doses Caused by a Hypothetical Reactor Accident, ORNL-TM-4082, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN.

AIRDOS

Model Type:	Dose from Atmospheric Pathways
Author:	R.E. Moore Health and Safety Research Division Oak Ridge National Laboratory Oak Ridge, TN 37830
Sponsoring Agency:	USEPA
Description:	AIRDOS estimates radionuclide concentrations in air, deposition rates, surface concentrations and individual or population doses from inhalation and ingestion. Atmospheric transport is calculated by a modified Gaussian plume model. Dose pathways include immersion in air and water, exposure to contaminated ground surfaces, inhalation and ingestion.
Review Reference:	SAI, SCEPTER, NS
Documentation:	Kaye, S.V., et al., 1973. Environmental Hazards Studies, Environmental Sciences Division Annual Progress Report ORNL-4935, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, September, p.1. Moore, R.E., 1975. AIRDOS: A Computer Code for Estimating Population and Individual Doses Resulting from Atmospheric Releases of Radionuclides from Nuclear Facilities, ERDA Report ORNL-TM-4687, Union Carbide Corporation, Oak Ridge National Laboratory, Oak Ridge, TN, January. Oak Ridge National Laboratory, 1979. AIRDOS-EPA: A Computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionuclides, ORNL-5532, Oak Ridge, TN.

AIREM

Model Type: Dose from Atmospheric Pathway

Author: J.A. Martin, Jr., C.B. Nelson and P.A. Cuny
U.S. Environmental Protection Agency
401 M Street, S.W.
Washington, DC 20460

Sponsoring Agency: USEPA

Description: AIREM was developed to estimate air concentrations, ground depositions (wet and dry) and external and inhalation doses resulting from emissions of nuclear fuel cycle facilities. The atmospheric transport portion of the model is based on a sector-averaged Gaussian plume model.

Review Reference: SAI, SCEPTER, NS

Documentation: Martin, J.A., Jr., C.B. Nelson and P.A. Cuny, 1974. AIREM Program Manual: A Computer Program for Calculating Doses, Population Doses, and Ground Deposition Due to Atmospheric Emissions of Radionuclides, EPA-5201/-74-004, Office of Radiation Programs, U.S. Environmental Protection Agency, Washington, DC, May.

AIRWAY

Model Type: Dose from Atmospheric Pathway

Author: J.L. Rider and S.K. Beal
Bettis Atomic Power Laboratory
P.O. Box 79
West Mifflin, PA 15122

Sponsoring Agency: USDOE

Description: AIRWAY calculates the dose commitment to man resulting from immersion in the plume, exposure to contaminated ground, inhalation of gaseous and suspended radioactivity. Air and ground concentrations of both the parent and daughter products are calculated. Atmospheric transport is calculated using a Gaussian plume model.

Review Reference: SAI, SCEPTER

Documentation: National Technical Information Service, WAPD-TM-1273, U.S. Department of Commerce, Springfield, VA, 34 pp.

AISITE II

Model Type: Dose from Atmospheric Pathway

Author:
R.A. Blaine
Mathematical and Computer Sciences
Atomics International
P.O. Box 309
Canoga Park, CA 91304

Sponsoring Agency: Unknown

Description: AISITE II was developed for the purpose of determining allowable sitings for nuclear reactors based on the siting criteria of NCR's 10CFR 100 regulations. The program can automatically vary up to 46 parameters describing the reactor operation. Doses are calculated as a function of distance for any organ or the critical organ with the fractional contribution by each isotope group being identified.

Review Reference: SAI, SCEPTER, NS

Documentation: Blaine, R.A. and E.L. Bramblett, 1964. AISITE II, A Digital Computer Program for Investigtion of Reactor Siting, NAA-SR-9982, Atomics International, September.

AREAC

Model Type: Dose from Atmospheric Pathway

Author:
D. Michlewicz
U.S.E.P.A. Office of Radiation Programs
401 M Street, S.W.
Washington, DC 20460

Sponsoring Agency: USEPA

Description: AREAC was designed to calculate radionuclide concentrations, population doses and individual inhalation doses resulting from atmospheric releases of radionuclides from area sources. The model accounts for cloud diffusion, ground and inverse lid reflections, radionuclide decay and area source shape.

Review Reference: SAI

Documentation: D. Michlewicz, 1976. ORP/EAD-76/6, Office of Radiation Programs, U.S. Environmental Protection Agency, Washington, DC, October, p. 63.

ARTRAN

Model Type:	Dose from Atmospheric Pathway
Author:	W.L. Dotson Hanford Engineering Development Laboratory P.O. Box 1970 Richland, WA 99352
Sponsoring Agency:	USAEC
Description:	ARTRAN is a submodel of the HERMES systems model designed to describe the air transport of radionuclides. Input data include source-receptor distance, effluent characteristics and meteorlogical variables. The code uses standard mathematial models for diffusion, deposition and transport.
Review Reference:	SAI, documentation below
Documentation:	Fletcher, J.L., and W.L. Dotson, 1971. HERMES: A Digital Computer Code for Estimating Regional Radiological Effects from the Nuclear Power Industry, HELD-TME-71-168, Hanford Engineering Development Laboratory, December Owen, P.T., et al. An Inventroy of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p.260.

BELCH

Model Type: Dose from Atmospheric Pathway

Author: Rodican P. Reed
Environmental Planning
Tennessee Valley Authority
River Oak Building
Muscle Shoals, AL 35660

Sponsoring Agency: Tennessee Valley Authority

Description: BELCH was designed to calculate individual and population doses from routine radioactive releases from power reactors. BELCH is based on NRC Regulatory Guides 1.109 and 1.111. The code calculates various organ doses for different spatial locations, for example, Gamma and Beta air doses at the site boundary, skin and total body at the nearest residence and thyrod doses at the nearest milk cow location.

Review Reference: SAI, SCEPTER

Documentation: Owen P.T., et al. An Inventory of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p.96.

2BPUFF

Model Type: Dose from Atmospheric Pathway

Author: K. Peterson
Lawrence Livermore Laboratory, L-262
G. Div, Physics Department
P.O. Box 808
Livermore, CA 94550

Sponsoring Agency: Unknown

Description: 2BPUFF calculates the dispersion of pollutants in a cylindrical cloud. Horizontal diffusivity is calculated using similarity theory of atmospheric turbulence while vertical diffusivity is entered as a function of height and time. The program considers wet and dry deposition and calculates cloud center and surface air concentrations as well as individual doses for a variety of pathways and nuclides.

Review Reference: SAI

Documentation: Owen P.T., et al. An Inventory of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p.79.

COMRADEX-IV

Model Type: Dose from Atmospheric Pathway

Author: E.R. Specht, J.M. Otter, and R.S. Hart
Rockwell International
Atomics International Division
P.O. Box 309
Canoga Park, CA 91305

Sponsoring Agency: Unknown

Description: COMRADEX-IV (Containment and meteorology of environmental radiation exposure) was developed to calculate the site dose resulting from the accidental radioactive release from a reactor. The program can be used to investigate the effect of filtration (by isotope), shielding, and varying leakage and fallout rates. The program uses either the Gaussian plume model of Pasquill or site specific attenuation factors. Dry deposition and radioactive decay are both considered. Dose calculations include direct gamma from the containment building, external gamma and beta from the cloud and internal inhalation doses to as many as 12 organs.

Review Reference: SAI, SCEPTER, NS

Documentation: Spangler, G.W., et al., 1967. Description of the COMRADEX Code, AI-67-TDR-108, McDonnell Douglas Corporation, Santa Monica, CA.

CRAC

Model Type:	Dose from Atmospheric Pathway
Author:	See Reference
Sponsoring Agency:	Unknown
Description:	CRAC was developed to calculate airborne concentrations and ground deposition of radionuclides released from a nuclear power accident. Health effect (dosimetric and dose response) were also included. The program is based on a Gaussian plume model with simplistic submodels to treat plume rise, inversion layers and rainstorms while wind shear and wind direction are not considered.
Review Reference:	SAI
Documentation:	Spring, J.L. et al., 1978. Investigations of the Adequacy of the Meteorological Transport Model Developed for the Reactor Safety Study, SAND77-1383C, paper presented at a conference on Probabilistic Analysis of Nuclear Reaction Safety, Los Angeles, CA, May 8. U.S. Nuclear Regulatory Commission, 1975. Reactor Safety Study: An Assessment of Accident Risks in the U.S. Commerical Nuclear Power Plants, WASH-1400 (NUREG-75/014), Washington, DC.

CUEX, AIRMOD

Model Type:	Dose from Atmospheric Pathway
Author:	D.C. Parzyck, J.F. Witherspoon and J.E. Till Environmental Sciences Division Oak Ridge National Laboratory Oak Ridge, TN 37830
Sponsoring Agency:	USDOE
Description:	CUEX (Cumulative Exposure Index) was developed to estimate radiation exposures resulting from environmental releases of radioactivity. CUEX is comprised of an atmospheric dispersion model AIRMOD and a terrestial transport model TERMOD.
Review Reference:	SAI
Documentation:	Parzyck, D.C., J.F. Witherspoon and J.E. Till. Validation of Environmental Transport Models in the CUEX Methodology, ORNL ESD Publication #1109, Oak Ridge National Laboratory, Oak Ridge, TN.

DACRIN

Model Type: Dose from Atmospheric Pathway

Author:
Dennis L. Strenge
Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: DACRIN can be used to calculate the dose to the human respiratory tract and other organs resulting from the inhalation of radioactive aerosols. The model is based on the ICRP Task Group Lung Model and doses can be calculated by either specifying the amount inhaled or through the use of a Gaussian plume dispersion model. Exposures can be either chronic or acute.

Review Reference: SAI, SCEPTER, NS

Documentation: Houston, J.R. D.L. Strenge and E.C. Watson, 1974. DACRIN - A Computer Program for Calculating Organ Dose from Acute or Chronic Radionuclide Inhalation, BNWL-B-389, Battelle Pacific Northwest Laboratories, Richland, WA, December.

Miller, C.W., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL - 5382, Oak Ridge National Laboratory, Oak Ridge, TN, June, p. 124.

Shriner, C.R. and L.J. Peck, 1978. Inventory of Data Bases, Graphics Packages, and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November, p. 206.

Strenge, D.L., 1975. DACRIN - A Computer Program for Computing Organ Dose from Acute or Chronic Radionuclide Inhalation: Modification of Gastroninterestinal Tract Dose, BNWL-B-389 SUPP, Battelle Pacific Northwest Laboratories, Richland, WA, February.

DOSE

Model Type: Dose from Atmospheric Pathway

Author: G.P. Kenfield
Atomics International
Canoga Park, CA 91304

Sponsoring Agency: Unknown

Description: DOSE was developed to calculate external and internal radiation doses from air releases of nuclear reactors. The model uses a fission product inventory (possibly obtained from an affiliated code CURIE) to calculate the dose to 14 internal organs. Dispersion is calculated using Suttons equation.

Review Reference: SAI

Documentation: Ellison, T.W. and A.B. Dunham. DOSE B: A CDC 6600 Program for Calculation of Inhalation and External Dose for Establishing Reactor Siting Distance Requirements, USAEC Report KAPL-M-6592, Knolls Atomic Power Laboratory, January.

Kenfield, G.P. et al, 1965. Curie-DOSE-THUNDERHEAD: A Digital Computer Program for External and Internal Radiation Dose Calculations, USAEC Report NAA-SR-8884, Atomics International, Canoga Park, CA.

Miller, C.W., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June.

GTC

EGAD

Model Type:	Dose from Atmospheric Pathway
Author:	R.E. Cooper Savannah River Laboratory Aiken, SC 29801
Sponsoring Agency:	USDOE
Description:	EGAD was developed to calculate the whole body dose resulting from atmospheric exposure of airborne radionuclides. The dispersion model assumes the cloud is bounded vertically between the ground and an upper inversion boundary and horizontally along the sector boundaries. The model is based on a Gaussian plume model.
Review Reference:	SAI, SCEPTER, NS
Documentation:	Cooper, R.E., 1972. EGAD - A Computer Program to Compute Dose Integrals from External Gamma Emitters, DP-1304, E.I. DuPont de Nemours & Co., Savannah River Laboratory, Aiken, SC. Miller C.W., et al. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June, p. 116.

EXDOSE

Model Type: Dose from Atmospheric Pathway

Author: M.M. Hendrickson
Battelle Pacific Northwest Laboratories
Richland, WA 99352

Sponsoring Agency: USDOE

Description: EXDOSE was developed to calculate the external gamma doses to the total body resulting from accidental releases of radionuclides. The code is based on a bivariate normal mode and Suttons equation. Ground deposition and radioactive decay/generation are included.

Review Reference: SAI, SCEPTER, NS

Documentation: Hendrickson, M.M. 1968. EXDOSE: A Computer Program Calculating the External Gamma Dose from Airborne Fission Products, USAEC Report BNWL-811, Battelle Pacific Northwest Laboratories, September.

Miller, C.W., et al., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June, p. 126.

EXGAM

Model Type: Dose from Atmospheric Pathway

Author: J.J. Steyn and Y.S. Kim
NUS Corporation
1730 M Street, N.W.
Washington, DC 20036

Sponsoring Agency: Unknown

Description: EXGAM was developed to calculate the gamma dose from an airborne release of radioactivity. The model is a Gaussian plume model and considers such factors as air attenuation and buildup.

Review Reference: SAI, SCEPTER, NS

Documentation: Owen P.T., et al. An Inventory of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p. 110.

Steyn, J.J. and Y.S. Kim, 1966. User's Manual for the Code EXGAM: A Code to Calculate Gamma Photon Dose from an Airborne Radioactive Release, USAEC Report NUS-329, Nuclear Utilities Services Corporation, November.

EXREM III

Model Type: Dose from Atmospheric Pathway

Author: D.K. Trubey and S.V. Kaye
Union Carbide Corporation
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, TN 37830

Sponsoring Agency: Unknown

Description: EXREM III is a modified version of EXREM a code that calculates external radiation exposure from submersion in contaminated air and water and exposure to contaminated surfaces. EXREM III calculates the contribution of daughter products in addition to parent nuclides. These models must interface with a model to provide nuclide concentrations. Contributions from gamma rays, x-rays, position and electron and beta radiations are all included in the dose calculations.

Review Reference: SAI, SCEPTER, NS

Documentation: Trubey, D.K. and S.V. Kaye, 1969. The EXREM III Computer Code for Estimating External Radiation Doses to Populations from Construction of a Sea-Level Canal with Nuclear Explosives, CTC-8, Union Carbide Corporation, Oak Ridge, TN.

Trubey, D.K and S.V. Kaye, 1973. The EXREM III Computer Code for Estimating External Radiation Doses to Populations from Environmental Releases, USAEC Report ORNL-TM-4322, Oak Ridge National Laboratories, December.

Turner, W.D., S.V. Kaye and P.S. Rohwer, 1968. EXREM and INREM Computer Codes for Estimating Radiation Doses to Populations from Constructioin of a Sea-Level Canal with Nuclear Explosives, K-1752, Union Carbide Corporation, Oak Ridge, TN.

FISSP/CLOUD

Model Type: Dose from Atmospheric Pathway

Author: L.L. Bonzon and J.B. Rivard
Sandia National Laboratories
Albuquerque, NM 87185

Sponsoring Agency: USDOE

Description: FISSP (Fission Product) and CLOUD were designed to be used jointly to estimate internal and external doses from atmospheric releases of radionuclides from nuclear reactors. CLOUD performs the atmospheric transport simulations using a Gaussian dispersion equation with Sutton's dispersion parameter. Dose resulting from both beta and gamma radiations are considered.

Review Reference: SAI

Documentation: Bonzon, L.L. and J.B. Rivard, 1970. Computational Method for Calculation of Radiological Dose Resulting from Hypothetical Fission Product Release, SC-RR-70-338, Sandia Laboratories, Albuquerque, NM.

Burkholder, H.C., J. Greenborg, J.A. Stottleyre, D.J. Bradley, J.R. Raymond and R.J.Serne, 1979. Waste Isolation Safety Assessment Program, Technical Progress Report for FY-77, PNL-2642/UC-70, Battelle Pacific Northwest Laboratory, Richland, WA, April, p. B-46.

GADOSE/DOSET

Model Type: Dose from Atmospheric Pathway

Author: E. Lee
General Atomic Company
San Diego, CA 92112

Sponsoring Agency: USDOE

Description: GADOSE was designed to calculate the radioactivity within a reactor plant and the doses to the public resulting from accidental instantaneous releases of radioactivity. The model includes the effects of decay, build up, filtration, atmospheric dilution, fallout and washout. DOSET was developed to consider the effect of a time dependent accidental fission product release.

Review Reference: SAI, SCEPTER, NS

Documentation: Lee, E. R.J. Mack and D.B. Sedgley, 1966. GADOSE and DOSET: Programs to Calculate Environment Consequences of Radioactivity Release, USEAEC Report GA-6511, General Atomic, April.

Miller, C.W., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report, April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June, p. 138.

GAMMA

Model Type: Dose from Atmospheric Pathway

Author: C.V. Gogolak
Environmental Measurements Laboratory
U.S. Department of Energy
376 Hudson Street
New York, NY 10014

Sponsoring Agency: USDOE

Description: GAMMA was developed to determine noble gas plume exposures from nuclear reactors. The model calculates atmospheric transport using a cross-wind averaged Gaussian plume and vertical dispersion coefficients of Watson and Gammerts folder. Decay and generation of radionculides is considered but deposition and inhalation are not.

Review Reference: SAI, SCEPTER, NS

Documentation: Owen, P.T., et al. An Inventory of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p.34.

GAUCHE

Model Type: Dose from Atmospheric Pathway

Author: D. Brenchley, J. Soldat, J. McNeese and E. Watson
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: GAUCHE can be used to calculate annual doses and in some cases dose commitments. Three pathways are considered, atmospheric submersion, inhalation and ingestion.

Review Reference: SAI

Documentation: Brenchley, D.L., J.K. Soldat, J.A. McNeese and E.C. Watson, 1977. Environmental Assessment Methodology for the Nuclear Fuel Cycle, BNWL-2219, Battelle Pacific Northwest Laboratories, Richland, WA, July.

GTC

GRONK

Model Type: Dose from Atmospheric Pathway

Author: J. Soldat, N.M. Robinson and D.A. Baker
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: GRONK (Gas Release of Nuclides) is a submodel of the HERMES systems model. This code calculates the annual dose resulting from the atmospheric release of radionuclides. Individual skin and total body doses as well as population total body dose can be calculated. The program uses either the Pasquill or Hanford dispersion models. Thyroid dose due to inhalation and ingestion of milk and leafy vegetables may be calculated.

Review Reference: SAI, SCEPTER, NS

Documentation: Burkholder, H.C., J. Greenborg, J.A. Stottlemyre, D.J. Bradley, J.R. Raymond and R. J. Serne, 1979.. Waste Isolation Safety Assessment Program, Technical Progress Report for FY-77, PNL-2642, Battelle Pacific Northwest Laboratories, Richland, WA, April, pp. B-39, 40.

Soldat, J.K., N.M. Robinson and D.A. Baker, 1974. Models and Computer Codes for Evaluating Environmental Radiation Doses, USAEC Report BNWL-1754, Battelle Pacific Northwest Laboratories, Richland, WA, February.

INDOS

Model Type: Dose from Atmospheric Pathway

Author: G.G. Killough and P.S. Rohwer
Health and Safety Research Division
Building 7509
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: INDOS is a series of computer codes that can be used to calculate the dose and dose rate to an organ as a function of time. Both inhalation and ingestion pathways are considered.

Review Reference: SAI, SCEPTER, NS

Documentation: Killough G.G. and P.S. Rohwer, 1974. INDOS: Conversational Computer Codes to Implement ICRP-10-10A Models for Estimation of Internal Radiation Dose to Man, ORNL-4916, Oak Ridge National Laboratory, Oak Ridge, TN.

Miller, C.W., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June.

Thykier-Nielsen, S., 1974. Models for Calculation of External Gamma Doses and Inhalation Doses from Releases of Radioactive Isotopes to the Atmosphere, RISO-M-1727, Danish Atomic Energy Commission, July (in Danish).

INGDOS

Model Type: Dose from Atmospheric Pathway

Author: J.C. Pleasant
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: INGDOS was developed to daclculate the organ dose resulting from the ingestion of food contaminated by atmospherically released radionuclides. The model is based on U.S.N.R.C. Regulatory Guide 1.109 for calculation of airborne radionuclides in food and annual doses to various organs resulting from ingestion. The model calculates nuclide concentrations in and on vegetation based on deposition velocity.

Review Reference: SAI

Documentation: Pleasant, J.C., 1979. INGDOS - A Conversational Computer Code to Implement U.S. Nuclear Regulatory Commission Regulatory Guide 1.109 Models for Estimation of Annual Doses from Ingestion of Atmospherically Released Radionuclides in Foods, ORNL-6571, Oak Ridge National Laboratory, Oak Ridge, TN, August.

GTC

KRONIC

Model Type: Dose from Atmospheric Pathway

Author: Dennis L. Strenge
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: KRONIC can be used to calculate the annual external total body dose resulting from the chronic release of radionuclides to the atmosphere. Atmospheric transport is calculated for multiple sectors using a standard plume dispersion approach. Both photon and beta particle contributions to the total dose are considered. Gamma dose can be calculated at any specified tissue depth.

Review Reference: SAI, SCEPTER, NS

Documentation: Arnett, R.C., R.A. Deju, R.W. Nelson, C.R. Cole and R.E. Gephart, 1976. Conceptual and Mathematical Modeling of the Hanford Groundwater Flow Regime, ARH-ST-140, Atlantic Richfield Hanford Company, Richland, WA, October.

Shiner, C.R. and L.J. Peck, 1978. Inventory of Data Bases, Graphics Packages and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November.

Strenge, D.L. and E.C. Watson, 1973. KRONIC - A Computer Program for Calculating Annual Average External Doses from Chronic Atmospheric Releases of Radionuclides, BNWL-B-264, Battelle Pacific Northwest Laboratories, Richland, WA.

MESODIF-II

Model Type: Dose from Atmospheric Pathway

Author/Contact: D.C. Powell, H.L. Wegley and T.D. Fox
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: MESODIF II was developed to calculate ground level air concentrations and deposition of effluents from nuclear power reactors. The model is a variable trajectory plume segment transport model that includes the effects of deposition. The model does not consider decay.

Review Reference: SAI, NS

Documentation: Pfuderer, H. and C. Johnson. 1979. Data Search Performed by Oak Ridge National Laboratory, Oak Ridge, TN, September.

Start, G.E. and L.L. Wendell, 1974. Regional Effluent Dispersion Calculations Considering Spatial and Temporal Meteorological Variations, NOAA Techn. Memo ERL-ARL-44, National Oceanographic and Atmospheric Administration.

NUBE

Model Type: Dose from Atmospheric Pathway

Author: A. Alonso
Junta de Energia Nuclear
Madrid, Spain

Sponsoring Agency: Unknown

Description: NUBE was developed to assess accidental releases of radionuclides from nuclear power plants. The model calculates the fission product inventory as a function of the reactor operating characteristics and calculates the atmospheric transport and subsequent individual, external and inhalation doses. Atmospheric transport processes include diffusion, condensation and deposition.

Review Reference: SAI, NS

Documentation: Alonso, Al, 1965. NUBE: A Digital Code to Evaluate the Hazards of Different Types of Reactor Accidents, International Symposium on Fission Product Release and Transport Under Accident Conditions, April 5-7, 1965, CONF-650407, Oak Ridge National Laboratory, Oak Ridge, TN, pp. 1080-1090.

PREDO

Model Type: Dose from Atmospheric Pathway

Author: Dennis L. Strenge
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: PREDO is a combination of the codes SITMET and WCLIM. SITMET uses hourly, onsite meteorological data to generate total body and/or skin doses for specified release inventories, release heights, and downwind distances. WCLIM generates a statistical distribution of doses with magnitude and direction.

Review Reference: SAI

Documentation: Owen, P.T., et al. An Inventory of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p. 289.

RACER

Model Type: Dose from Atmospheric Pathway

Author: D.L. Strenge, M.M. Hendrickson and E.C. Watson
Battelle Pacific Northwest Laboratories
Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: RACER was developed to calculate the tissue dose resulting from gamma radiation emitted by airborne radionuclides. Atmospheric transport is simulated using a Gaussian plume model with decay/generation of radionuclides considered. Organ dose resulting from inhalation is not considered.

Review Reference: SAI, NS

Documentation: Burkholder, H.C., J. Greenburg, J.A. Stottlemyre, D.J. Bradley, J.R. Raymond, and R.J. Serne, 1979. Waste Isolation Safety Assessment Program Technical Progress Report for FY-77, PNL-2642, Pacific Northwest Laboratory, Richland, Wa, p. B-50, April.

Gumprecht, R.O., 1968. Mathematical Basis of Computer Code RIBD, RUN-4136, Douglas United Nuclear, Inc., Richland, WA.

Gumprecht, R.O., 1969. Computer Code RIBD, DUN-SA-69, Douglas United Nuclear, Inc., Richland, WA.

Strenge, D.L., M.M. Hendrickson and E.C. Watson, 1971. RACER: A Computer Program for Calculating Potential External Dose from Airborne Fission Products Following Postulated Reactor Accidents, BNWL-B-69, Battelle Pacific Northwest Laboratories, Richland, WA.

RADOS

Model Type:	Dose from Atmospheric Pathway
Author:	R.E. Cooper Savannah River Laboratory Aiken, SC 29801
Sponsoring Agency:	USDOE
Description:	RADOS was developed to calculate the total body gamma dose from a cloud of air borne material. The model assumes instantaneous release and a cloud of unit thickness in the downwind direction. Dispersion is based on a Gaussian model.
Review Reference:	SAI, SCEPTER, NS
Documentation:	Cooper, R.E., 1968. RADOS - A Code to Estimate Gamma Dose from a Cloud of Radioactive Gases, USAEC Report DP-1098, E.I. DuPont de Nemours and Co., Savannah River Laboratory, Aiken, SC, June. Shriner, C.R. and L.J. Peck, 1978. Inventory of Data Bases, Graphics Packages and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November.

RSAC-2

Model Type: Dose from Atmospheric Pathway

Author/Contact: R.L. Coates, N.R. Horton and L.C. Richardson
National Reactor Testing Station
Idaho Falls, ID 83401

Sponsoring Agency: USDOE

Description: RSAC-2 can be used to calculate the radiological consequences of an accidental release of radionuclides to the atmosphere. Specifically the model can calculate fission product inventroy, lung doses, gastrointestinal tract doses, internal organ dose, gamma doses due to ground deposition and air suspension. Atmospheric concentrations are calculated using a bivariate normal distribution model.

Review Reference: SAI, SCEPTER, NS

Documentation: Burkholder, H.C. J. Greenborg, J.A. Stottlemyre, D.J. Bradley, J.R. Raymond and R. J. Serne, 1979.. Waste Isolation Safety Assessment Program, Technical Progress Report for FY-77, PNL-2642, Battelle Pacific Northwest Laboratories, Richland, WA, April, pp. B-53.

Coates, R.L. and N.R. Horton, 1966. RSAC: A Radiological Safety Analysis Computer Code, U.S. AEC Report IDO-17151, Phillips Petroleum Company, National Reactor Testing Station, Idaho Falls, ID.

Dolphin, G.W. and I.S. Eve, 1966. Dosimetry of the Gastrointestinal Tract, Health Physics, Vol. 12, pp. 163-172.

International Commission on Radiological Protection, 1959. ICRP Publication 2, Pergamon Press, Oxford.

International Commission on Radiological Protection, 1964. ICRP Publication 6, Pergamon Press, Oxford.

Richardson, L.C., 1968. User's Manual for the FORTRAN Version of RSAC, a Radiological Safety Analysis Computer Program, U.S. AEC Report IDO-17261, Phillips Petroleum Company, National Reactor Testing Station, Idaho Falls, ID.

Wenzel, D.R., 1974. A Computer Code to Calculate Doses Resulting from Release of Radionuclides to the Atmosphere, Health Physics, Vol. 27, p. 641 (abstract).

STAREL/RELISH

Model Type: Dose from Atmospheric Pathway

Author: F.T. Binford
Oak Ridge National Laboratory
Operations Divison
P.O. Box X
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: STAREL was developed to calculate ground level concentrations from a series of stacks. RELISH calculates isopaths for the stack releases in various co-ordinate systems.

Review Reference: SAI, SCEPTER, NS

Documentation: Binford, F.T., T.P. Hamrick and B.H. Cope, 1970. Some Techniques for Estimating the Results of the Emission of Radioactive Effluent from ORNI Stacks, USAEC Report ORNL-TM-3613, Oak Ridge National Laboratory, Oak Ridge, TN, October.

Owen, P.T., et al. An Inventroy of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p. 128.

SUBDOSA

Model Type: Dose from Atmospheric Pathway

Author: D.L. Strenge
Battelle Pacific Northwest Laboratory
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: SUBDOSA was developed to calculate the external dose to humans following accidental atmospheric releases of radionuclides. Spatial distribution of radionuclides is calculated based on source strength, duration, atmospheric conditions and distance to receptor. Dose is calculated for skin, eyes, gonads, and total body. Inhalation is not considered.

Review Reference: SAI, SCEPTER, NS

Documentation: Shriner, C.R. and L.J. Peck, 1978. Inventroy of Data Bases, Graphics Packages and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November.

Strenge, D.L., E.C. Watson and J.R. Houston, 1975. SUBDOSA: A Computer Program for Calculating External Doses from Accidental Atmospheric Releases of Radionuclides, ERDA Report BNWL-B-351. Battelle Pacific Northwest Laboratories, Richland, WA.

SUBPOPA

Model Type: Dose from Atmospheric Pathway

Author: D.L. Strenge
Battelle Pacific Northwest Laboratory
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: SUBPOPA can be used to calculate the population dose from beta and gamma radiations resulting from accidental releases of radionuclides to the atmosphere. Transport through the atmosphere is represented by the joint frequency distribution of wind vector and atmospheric stability. Radioactive decay is considered. Release duration is assumed to be one hour.

Review Reference: SAI, SCEPTER, NS

Documentation: Burkholder, H.C., J. Greenburg, J.A. Stottlemyre, D.J. Bradley, J.R. Raymond and R.J. Serne, 1979. Waste Isolation Safety Assessment Program, Technical Progress Report for FY-77, PNL-2642/UC-70, Battelle Pacific Northwest Laboratories, Richland, WA, April, p. B-56.

Shriner, C.R. and L.J. Peck, 1978. Inventory of Data Bases, Graphics Packages and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November, p.208.

THUNDERHEAD

Model Type: Dose from Atmospheric Pathway

Author: G.P. Kenfield
Atomics International
Canoga Park, CA 91304

Sponsoring Agency: Unknown

Description: THUNDERHEAD uses fission product activity data from CURIE to calculate the external cloud gamma exposure from the released fission products.

Review Reference: SAI, SCEPTER, NS

Documentation: Kenfield, G.P., et al., 1965. CURIE-DOSE-THUNDERHEAD: A Digital Computer Program for External and Internal Radiation Dose Calculations, USAEC Report NAA-SR-8884, Atomics International, Canoga Park, CA.

Miller, C.W., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June.

UDAD

Model Type: Dose from Atmospheric Pathway

Author: M.H. Momeni
Argonne National Laboratory
Environmental Impact Studies Division
9700 South Cass Avenue
Argonne, IL 60439

Sponsoring Agency: USDOE

Description: UDAD (Uranium Dispersion and Dosimetry) was developed to estimate the radiological and health effects arising from uranium mining and milling operations. The model can be used to calculate airborne concentrations, ground deposition, dose rates and doses from emissions. Air concentrations are calculated using an annually averaged Gaussian diffusion model. Cloud depletion through deposition and decay is considered.

Review Reference: SAI

Documentation: Momeni, M.H. et al., 1979. The Uranium Dispersion and Dosimetry (UDAD) Code, NUREG/CR-0553 (ANL/ES-72), Argonne National Laboratory, prepared for the U.S. Nuclear Regulatory Commission, Washington, DC, May.

Owen, P.T., et al. An Inventory of Environmental Impact Models Relating to Energy Technologies, ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN, p. 270.

VITTLS

Model Type: Dose from Atmospheric Pathway

Author: D.L. Brenchley, J.K. Soldat, J.A. McNeese, and E.C. Watson
Battelle Pacific Northwest Laboratories
Richland, WA 99352

Sponsoring Agency: USDOE

Description: VITTLS calculates radionuclide concentrations on soil resulting from aerial deposition or irrigation. These calculations are then used to calculate individual annual dose and dose commitments to skin and total body. Organ doses resulting from ingestion are also considered.

Review Reference: SAI

Documentation: Brenchley, D.L., J.K. Soldat, J.A. McNeese and E.C. Watson, 1977. Environmental Assessment Methodology for the Nuclear Fuel Cycle, BNWL-2219, Battelle Pacific Northwest Laboratories, Richland, WA, July.

WRED

Model Type: Dose from Atmospheric Pathway

Author: R.E. Cooper
Savannah River Laboratory
E.I duPont de Nemours and Co.
Aiken, SC 29801

Sponsoring Agency: Unknown

Description: WRED is a reactor siting code designed to estimate probability distributions of wholebody gamma and thyroid doses using measured meteorological parameters as input data.

Distribution analyses are performed as a function of downwind distance, activity release height and wind direction. This statistical approach for gamma dose estimates, employing thousands of sets of meteorology data, is accomplished using two-dimensional tables of space distribution-attenuation intergrals and interpolation techniques.

Review Reference: SAI, NS

Documentation: Cooper, R.E., 1969. WRED: A Siting Code to Estimate Dose Probability Distribution from Measured Meteorolgy Data, Health Physics, Vol. 16, pp. 735-738.

Miller, C.W. et al, 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report, April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June, pp. 121-2.

XOQDOQ

Model Type:	Dose from Atmospheric Pathway
Author:	John Goll U.S. Nuclear Regulatory Commission Washington, DC
Sponsoring Agency:	USNRC
Description:	XOQDOQ was developed to calculate airborne concentrations and deposition values resulting from routine releases from nuclear power reactors. The model is based on NRC's Regulatory Guide 1.111.
Review Reference:	SAI, SCEPTER, NS
Documentation:	Science Applications, Incorporated. 1-013-71-800-02, Vol.1, Science Applications, Inc., La Jolla, CA.

DOSE FACTOR/HEALTH EFFECT MODELS

DARTAB

Model Type: Dose Factor/Health Effects

Author: D.E. Dunning, Jr., R.W. Leggett and M.G. Yalcintas
Oak Ridge National Labaoratory
Oak Ridge, Tennessee

Sponsoring Agency: USEPA

Description: DARTAB can be used to calculate the dose rate to a specific individual, average individual and the collective population dose. The model requires dose factors, risk factors and air intake and exposure data. Four main pathways ingestion, inhalation, air immersion and ground surface exposure are considered.

Review Reference: NRC (3)

Documentation: Dunning, D.E., Jr., Leggett, R.W., and Yalcintas, M.G. A Combined Methodology for Estimating Dose Rates and Health Effects from Radioactive Pollutants. ORNL/TM-7105. Oak Ridge National Laboratory. 1980.

DISDOS

Model Type: Dose Factor/Health Effects

Author: K. O'Brien
U.S. Atomic Energy Commission
New York, NY

Sponsoring Agency: USAEC

Description: DISDOS calculates the propagation of environmental gamma rays incident on the human body.

The propagation of environmental gamma rays through the human body is accounted for by using the three-dimensional Monte Carlo computer code, DISDOS. The radiation field was assumed to be isotropically incident. The calculation was performed with the aim of determining the dose to the body organs with a statistical accuracy of better than 10 percent.

Review Reference: SAI

Documentation: Miller, C.W., 1978. The Evaluation of Models Used for the assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN.

DOSHEM

Model Type: Dose Factor/Health Effects

Author: G.E. Runkle, R.M. Cranwell and J.D. Johnson
Sandia National Laboratories
Albuquerque, New Mexico

Sponsoring Agency: USNRC

Description: DOSHEM was developed to interface with the transport model PATH and to calculate the dose to man and associated health risks resulting from the inhalation, ingestion and exposure to radionuclides. The program combines the dose from each radionuclide to each organ for every pathway to calculate whole body and individual organ doses. Doses from all radionuclides in the inventory are summed and used to estimate increased risk of an individual dying of cancer. The model requires dose factors and risk factors as input parameters.

Review Reference: NRC (3)

Documentation: Runkle, G.E., Cranwell, R.M. and Johnson, J.D. Risk Methodology for Geologic Disposal of Radioactive Waste: Dosimetry and Health Effects. NUREG/CR-2166. SAND 80-1372 GF. Sandia National Laboratories. July 1981.

Runkle, G.E. and Cranwell, R.M. User's Manual for the Dosimetry and Health Effects Model, (Rough draft) Sandia National Laboratories, July 1981.

ICRP

Model Type: Dose Factor/Health Effects

Author: J.K. Soldat
Battelle Pacific Northwest Laboratoies
Richland, WA 99352

Sponsoring Agency: Unknown

Description: ICRP calculates the total annual dose and the 50 year dose commitment for various categories of people and integrates these doses for the population. Equations for calculating dose factors are based on those suggested by the ICRP (International Commission on Radiological Protection). Effective decay energies for various radionulcides were also based on the ICRP model.

Review Reference: SAI

Documentation: ICRP Task Group on Lung Dynamics, 1966. Deposition and Retention Models for Internal Dosimetry of the Human Respiratory Tract, Health Physics, Vol. 12, pp. 173-207.

International Commission on Radiological Protection, 1959. Report of ICRP Committee II on Permissible Dose for Internal Radiation, ICRP Publication 2, Pergamon Press, Oxford.

International Commission on Radiological Protection, 1968. Report of Committee IV on the Evaluation of Radiation Doses to Body Tissues from Internal Contamination Due to Occupational Exposure, ICRP Publication 10, Pergamon Press, New York.

Soldat, J.K., 1971. Modeling of Environmental Pathways and Radiation Doses from Nuclear Facilities, BNWL-SA-3939, Battelle Pacific Northwest Laboratories, Richland, WA.

IMPACT

Model Type: Dose Factor/Health Effects

Author: Robert McKee
Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352

Sponsoring Agency: USDOE

Description: IMPACT was developed to calculate annual and cumulative health impacts and the operating costs associated with a given waste management system. The model calculates the 70 year dose commitment for total body, bone, lungs and thyroid. Waste management cost calculations include treatment, interim storage, transportation and repository costs.

Review Reference: SAI

Documentation: U.S. Department of Energy, 1979. Technology of Commercial Radioactive Waste Management, DOE/ET-0028, Washington, DC, May.

GTC

INDOS

Model Type: Dose Factor/Health Effects

Author:
G.G. Killough and P.S. Rohwer
Health and Safety Research Division
Building 7509
Oak Ridge National Laboratory
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: INDOS calculates radiation doses to organs of the body based on ICRP-10-10-A models. The model calculates concentrations of airborne radionuclides in food and computes dose and dose rate to an organ as a function of time. Input to the model includes parameters describing the radionuclide and organ and the specification of a mathematical model.

Review Reference: SAI

Documentation:

Killough, G.G. and P.S. Rohwer, 1974. INDOS: Conversational Computer Codes to Implement ICRP-10-10A Models for Estimation of Internal Radiation Dose to Man, ORNL-4916, Oak Ridge National Labortary, Oak Ridge, TN.

Miller, C.W., 1978. The Evaluation of Models Used for the Assessment of Radionuclide Releases to the Environment (Progress Report April 1976 - December 1977), ORNL-5382, Oak Ridge National Laboratory, Oak Ridge, TN, June.

INREM, INREM II

Model Type: Dose Factor/Health Effects

Author:
G.G. Killough
Oak Ridge National Laboratory
Health and Safety Research Division
Building 7509
P.O. Box X
Oak Ridge, TN 37830

Sponsoring Agency: USDOE

Description: INREM can be used to estimate the cumulative dose to body organs due to inhalation or ingestion. Dose calculations are based on adaptations of model presented in ICRP Publication 2.

Review Reference: SAI

Documentation:

Killough, G.G., 1978. INREM II: A Computer Implementation of Recent Models for Estimating the Dose Equivalent to Organs of Man for an Inhaled or Ingested Radionuclide, NUREG-CR-0114, Oak Ridge National Laboratory, Oak Ridge, TN.

Killough, G.G., P.S. Rohwer, and W.D. Turner, 1975. INREM - A FORTRAN Code Which Implements ICRP 2 Models of Internal Radiation Dose to Man ORNL-5003, Environmental Sciences Division Publication No. 640, Oak Ridge National Laboratory, Oak Ridge, TN.

Shriner, C.R., and L.J. Peck, 1978. Inventory of Data Bases, Graphics Packages, and Models in Department of Energy Laboratories, ORNL/EIS-144, Oak Ridge National Laboratory, Oak Ridge, TN, November.

Turner, W.D., S.V. Kaye, and P.S. Rohwer, 1968. EXREM and INREM Computer Codes for Estimating Radiation Doses to Populations from Construction of a Sea-Level Canal with Nuclear Explosives, K-1752, Union Carbide Corporation, Oak Ridge, TN.

SYSTEMS MODEL SUMMARIES

Table 7. Summary of Systems Model Capabilities

Model	Author	Processes Addressed						Comments
		Source Term	G/W Flow & Transport	Surface Water Transport	Dose to Man			
					Inhalation	Ingestion	Exposure	
AMRAW	S.E. Logan USEPA	Uses ORIGEN	-presumably addressed in Release Model	-presumably addressed in Environmental Model	-program does calculate a dose but insufficient description given to identify mechanism			-some probabilistic elements with regards to risk analysis mode (i.e. events distributed probabilistically over time).
CALMRC	Blake Robertson NRC	-insufficient description	-uses AUTOMIG -solves 1-D transport for point sources in saturated media -does not consider generation	-insufficient description	-uses INHDOSE -Gaussian plume -gaseous and particulate -does not consider decay	-considers well contamination	-addressed	-calculates concentrations in disposal sites so that maximum allowable doses are not exceeded
HERMES	Fletcher and Dotson Atomic Energy Commission	-considers operational releases from both nuclear power plants and reprocessing plants	-insufficient description but probably too simplistic	-completely mixed cell approach	-both gaseous and particulate deposition -dose to body and 6 organs	-sophisticated food chain	-calculates annual radiation dose -also dose from immersion	-source term not applicable -considers multiple sources -surface and ground water probably too simplified -dose calculations may be useful
NRC Liquid Pathways Generic Study	D.L. Schreiber et al. USNRC	-calculations based on accident scenario at power plant	-2D analytical solution -1D surface water groundwater interface model	-1D analytical solutions for most surface water bodies -considers sediment and decay	-does not consider atmospheric transport or dose due to inhalation	-considers ingestion of water and aquatic foods	-considers exposure to contaminated sediment -immersion in water	-these models do not consider generation -sensitivity analysis and some validation has been conducted

Table 7 (Cont'd)

Model	Author	Processes Addressed						Comments
		Source Term	G/W Flow & Transport	Surface Water Transport	Dose to Man			
					Inhalation	Ingestion	Exposure	
NUTRAN	The Analytic Sciences Corp.	ORIGIN calculates inventory -leaching and dissolution included	-transport along 1-D flow paths using analytic solution	-mass transport, dilution diffusion, sedimentation are modeled by compartments and transfer coefficients	not considered	-considers water, aquatic foods, irrigated crops, farm animals -both population and individual -whole body and 7 organs -dose committment	-considers both water and soil	-g/w flow pathways can be probability dependent
PRESTO	C. A. Little et al. USEPA	-daughter products of long-lived decay chains not considered	-1-D streamlines using an analytic expression to account for decay and dispersion	-highly dependent on user-supplied coefficient -does not consider g/w component	-Gaussian transport suspension and deposition considered -calculates maximum, average and population dose commitments	-models irrigation and food chain, both aquatic and terrestrial	-both water and soil	-future versions will consider intrusion as well as operational scenarios
SYVAC	Dormouth and Quick AECL	-Bateman equations describe inventory -dissolution/leaching assumed to be a function of advection or diffusion -ignores initial transient phase	-based on steady-state advection of a three member chain along a 1-D streamline	-compartment model considers transients	-not considered	-both aquatic and terrestrial -assumed steady state	-requires compartment volumes and transfer coefficients	-specifically tailored for deep disposal of CANDU waste -all input parameters have user-defined prob. density functions for Monte Carlo simulations

Table 7 (Cont'd)

Model	Author	Processes Addressed						Comments
		Source Term	G/W Flow & Transport	Surface Water Transport	Dose to Man			
					Inhalation	Ingestion	Exposure	
NRC Sandia Risk Assessment Methodology	Various Authors USNRC	NWFT/DVM	NWFT/DVM	Environmental Model -compartment models with transfer coefficients (sub-model of PATH1)	Transport to Man Model -PATH1 submodel -ignores decay due to long half lives -both aquatic and terrestrial -considers resuspension	Transport to Man Model	-Uses DOSHEM -70 year dose commitment	-accuracy of model results will be highly dependent on user selection of transfer coefficient, concentration factors, etc.

AMRAW

Model Type: Systems Model

Author: S. E. Logan
S. E. Logan and Associates, Inc.
La Tierra Box 1054
Buckman Road
Santa Fe, NW 87501
U.S.A.

Sponsoring Agency: USEPA

Availability: Through author or NTIS

Programming:

(i) Language: FORTRAN
(ii) System: IBM 360

Description:

(i) Summary: AMRAW consists of two submodels AMRAW-A and AMRAW-B. AMRAW-A consists of a source term model which includes ORIGEN, a release model and an environmental model. The release model uses a risk analysis mode to describe events distributed probabilistically over time or a consequence analysis mode for discrete events occurring at specified times. The submodels are described as "being simple but attempting to account for essentials of the processes". The environmental model is a lumped parameter model where compartments are assumed to be completely mixed and transport is accounted for by transfer coefficients. This submodel includes the transport to and accumulation at various receptors in the biosphere, the pathways from these environmental concentrations and the resulting dose to man.

AMRAW-B is a cost/benefit model which calculates health effects in terms of economic costs corresponding to the various organ dose rates from AMRAW-A.

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(ii) Inputs: Not reported but presumably compartment volumes and transfer coefficients, waste inventory and system geometry.

(iii) Outputs: Not reported.

Validation: None reported.

Verification: None - model has been applied to a bedded salt reference repository and terminal storage in a shale repository.

Quality Assurance: None reported.

Review Reference: CEC, SAI, SCEPTER

Documentation: S. E. Logan and M.C. Berbano (1978). "Development and Application of a Risk Assessment Method for Radioactive Waste Management." Volumes I-IV, EPA 520/6-78-005 U.S. Environmental Protection Agency, Washington, DC.

CALMAC

Model Type: Systems Model

Author: Blake Robertson
Ford Bacon & Davis Utah
375 Chipeta Way
Salt Lake City UT 84108

Sponsoring Agency: USNRC

Availability: Through Author

Programming:

(i) Language: FORTRAN
(ii) System: UNIVAC 1108

Description:

(i) Summary: This model calculates allowable concentrations of nuclides in a disposal site so that maximum allowable doses are not exceeded. The model can consider up to 23 nuclides along a maximum of six exposure pathways and calculates the maximum average concentration of each nuclide. Pathways include well water contamination, inhalation and direct exposure with each pathway represented by analytical expressions which are solved algebraically. INHDOSE is a subprogram of CALMAC that calculates the atmospheric dispersion of gaseous and particulate emissions from areal and point sources. The code considers particle deposition as well as source strength related to wind speed. The decay of nuclides is generally not considered. AUTOMIG is another submodel that calculates the transport of nuclides using one-dimensional analytic solutions for point sources in saturated media. AUTOMIG requires fluid velocities as input. Generation of daughter products is not considered.

(ii) Inputs: not described in review reference

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(iii) Outputs: Not described in review reference.

Validation: None reported.

Verification: None reported.

Quality Assurance: None reported.

Review Reference: SAI

Documentation/ Reference : Adam, J.A., and V.L. Rogers, 1978. A Classification System for Radioactive Waste Disposal -- What Waste Goes Where? NUREG-0456, U.S. Nuclear Regulatory Commission, Washington, DC., June.

HERMES

Model Type: Systems Model

Author: J. F. Fletcher and W. L. Dotson
Hanford Engineering Development Laboratory
Richland, WA 99352

509-942-6523; FTS 444-6523

Sponsoring Agency: U.S. Atomic Energy Commission

Programming:

(i) Language: FORTRAN
(ii) System: CDC 7600

Description:

(i) Summary: HERMES simulates the regional radiological effects resulting from the operation of nuclear facilities to satisfy projected electrical energy requirements. The model uses a linear programming technique to determine the optimum mixture of generating facilities in the region under study. Each plant is assigned to a site based upon load centres and other criteria. A subroutine (MOPOSH) is used to determine monthly capacity factors based upon anticipated demand. Two other subprograms DOSIS and REPARE calculate expected effluents from power and reprocessing plants. This information is fed into a post procesor, RADEL, which transforms source characteristics and emission rates and develops a receptor map based on population and geographical data. Radionuclides are transported from their source by air and/or water transport. The air transport code (ARTRAN) uses monthly climatological data applied to standard mathematical models for diffusion, deposition and transport. The water transport code (WTRAN) calculates radionuclide concentrations of both dissolved and adsorbed onto sediments. Water concentrations are based on the assumption of completely mixed river compartments comprising a river basin.

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Sediment flow is based on an empirical equation requiring calibration to field data. Both surface run-off and groundwater contributions are addressed by the model, but little information describing these processes is given in the documentation. The submodel DOSE calculates both the total body dose and the dose to six organs (gastro-intestinal tract, bones, liver, thyroid, skin and lungs). The primary dose pathways considered are direct immersion, inhalation, external exposure and ingestion. The ingestion mechanism considers a number of food chain pathways (e.g., concentration effects), deposition on plant surfaces and incorporation into animal and plant tissues. Dose calculations are performed for three population age groups -- child, teenage and adult -- and consist of a 50-year dose commitment, annual radiation dose. Calculations are made for both average and maximum individuals in each category.

(ii) Inputs:

ARTRAN:
- source characteristics, e.g. height, emission rate, location
- receptor location
- meteorological data, e.g. mean, wind speed, mixing depths
- particulate characteristics, i.e., washout coefficient

DOSE:
- air, water concentration
- food transfer coefficients
- diet description
- crop yields
- population characteristics

WTRAN
- monthly stream flow
- radionuclide source in reach
- distribution coefficients
- sediment transport constants
- river basin characteristics

(iii) Outputs:

ARTRAN:
- spatial and temporal radionuclide concentrations and deposition patterns

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(iii) Outputs:	DOSE:	- whole body and organ dose for three age categories
	WTRAN:	- dissolved and adsorbed radionuclide concentrations in surface water bodies

Validation:	None reported.
Verification:	None reported.
Quality Assurance:	None reported.
Review Reference:	SAI; Fletcher, J.F., and W. L. Dotson, 1971. HERMES: A Digital Computer Code for Estimating Regional Radiological Effects from the Nuclear Power Industry, HEDL-TME-71-168, Hanford Engineering Development Laboratory, Richland, WA, 759 pp.
Documentation:	Fletcher, J.F., and W. L. Dotson, 1971. HERMES: A Digital Computer Code for Estimating Regional Radiological Effects from the Nuclear Power Industry, HEDL-TME-71-168, Hanford Engineering Development Laboratory, Richland, WA, 759 pp.

NRC-LPGS

Model Type: Systems Model

Authors: D. L. Schreiber, H. Berkson, G. L. Chipman, R. B. Codell, K. F. Eckerman, O. D. Lynch, A. R. Marchese, P. F. Riehm

Sponsoring Agency: USNRC

Availability: Portions still under development

Programming:

(i) Language: FORTRAN, BASIC
(ii) System: Unknown

Description:

(i) Summary: The NRC-Liquid Pathways Generic Study was undertaken by NRC to evaluate accident risks associated with floating nuclear power plants. Two types of accidents -- design basis accidents and core melt accidents -- were considered and models were developed for each type of scenario. The models developed for core-melt accidents are generally more realistic and for example, include the effects of sedimentation in surface water models. Processes considered in the study include ground water transport, surface water transport, ingestion, immersion and food concentration. The surface water models, although simplistic, consider most surface water configurations (e.g., lakes, rivers, oceans, great lakes, estuaries) and present solutions in the form of analytical equations. Radionuclide decay is considered. The ground water model consists of an analytical solution to transport in a two-dimensional aquifer with a point source. A ground water/surface water interface model (also in analytical form) can be used to calculate ground water contribution to surface water. Dose to man is calculated by summing the product of dose factors and integrated concentration over time for all pathways. Pathways considered include ingestion of water and aquatic foods, immersion (i.e., swimming) and direct exposure to contaminated sediment.

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(ii) Inputs: **Surface Water:**

- geometry, flow rates, input concentrations
- distribution coefficients
- decay rates
- channel properties, e.g., Mannings "n"

Ground Water:

- aquifer geometry
- g/w velocity

Dose:

- g/w consumption rate
- bioaccumulation factors
- dose factors
- pathway usage factors

(iii) Outputs: **Surface Water:**

- concentrations as a function of time and space

Ground Water:

- concentrations as a function of time and space

Dose:

- dose to individual and population

Validation: The sedimentation concentration in the Clinch and Tennessee Rivers has been calculated and compared to observed values. More recent documentation (NRC 1981) presents more detailed model "confirmation".

Verification: Not reported.

Quality Assurance: Not reported.

Review Reference: U.S. Nuclear Regulatory Commission. 1978a. Liquid Pathway Generic Study. Impacts of Accidental Radioactivity Releases to the Hydrosphere from Floating and Land-Based Nuclear Power Plants. NUREG-0440.

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Documentation/ Reference : U.S. Nuclear Regulatory Commission. 1981. A Collection of Mathematical Models for Dispersion in Surface and Groundwater. NUREG-0868.

NRC - Sandia Risk Assessment Methodology

Model Type: Systems Model

Author: Various - Sandia Laboratories
Albuquerque, New Mexico 87185

Sponsoring Agency: USNRC

Availability: Through NRC

Programming:

(i) Language: FORTRAN
(ii) System: CDC 176

Description:

(i) Summary: The Sandia Risk Assessment Methodology consists of a suite of models and statistical techniques for evaluating the long-term risks from radioactive waste disposal in deep geologic media. Source and ground water transport calculations are performed by NWFT/DVM. The source model in NWFT/DVM considers leach rates and individual radionuclide solubilities. The transport simulation in NWFT/DVM can treat decay chains with any number of daughter projects each having different distribution coefficients. The network flow model in NWFT/DVM allows simple 1-dimensional flow or quasi-two dimensional flow. The model can be used alone or in conjunction with a multidimensional flow. At Sandia, the SWIFT model is often used to provide boundary conditions for NWFT/DVM. SWIFT is a three-dimensional model that solves the flow and transport equations using a finite difference method. This permits the re-creation of the velocity field as a network of one-dimensional segments through which radionuclide transport is simulated. To link the ground water transport models to the biosphere, a pathways model was developed. This model consists of an Environmental Transport Model, which simulates the movement of radionuclides from the surface water through the food chain and

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a Transport to Man Model that calculates the potential quantity of nuclides through inhalation and ingestion. The Transport to Man Model and Environmental Transport Model comprise the PATH2 model and can be used to calculate concentrations of radionuclides inhaled or ingested by an individual. A dosimetry and health effects model (called DOSHEM by Mills and Vogt) can be used to calculate resulting dose to man.

(ii) Inputs: NWFT/DVM: flow system boundary conditions and properties, initial inventory, nuclide solubilities and distribution coefficients

PATH1: volume of compartments, Kd, concentration ratios, radionuclide input rates, agricultural parameters, ingestion inhalation patterns

DOSHEM: radionuclide concentrations for all pathways

(iii) Outputs: When used together, final output is in the form of doses to man and health effect calculations.

Verification: SWIFT, NWFT/DVM have been verified against analytical solutions.

Quality Assurance: Not reported.

Review Reference: M. Mills, D. Vogt. A Summary of Computer Codes for Radiological Assessment. NUREG/CR-3209.

G. E. Runkle, R. M. Cranwell, J. D. Johns. Risk Methodology for Geologic Disposal of Radioactive Wastes: Dosimetry and Health Effects. NUREG/CR-2166.

Documentation/ Reference: J. E. Campbell, R. T. Dillon, M. J. S. Tierney, H. T. Davis, P. E. McGrath, F. J. Pearson, Jr., H. R. Shaw, J. C. Helton, and F. A. Donath, 1978. Risk Methodology for Geolotic Disposal of Radioactive Waste: Interim Report, NUREG/CR-0458, SAND78-0029, Sandia Laboratories, Albuquerque, NM.

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J. E. Campbell, P. C. Kaestner, B. S. Langkopf and R. B. Lantz, 1980. Risk Methodology for Geologic Disposal of Radioactive Waste: The Network Flow and Transport (NWFT) Model, NUREG/CR-1190, SAND79-1920, Sandia National Laboratories, Albuquerque, NM.

R. T. Dillon, R. B. Lantz and S. B. Pahwa, 1978. Risk Methodology for Geologic Disposal of Radioactive Waste: The Sandia Waste Isolation Flow and Transport (SWIFT) Model, NUREG/CR-0424, SAND78-1267, Sandia National Laboratories, Albuquerque, NM.

J. C. Helton and P. C. Kaestner, 1981. Risk Methodology for Geologic Disposal of Radioactive Waste: User Manual Pathways Model, NUREG/CR-1636, SAND78-1711, Sandia National Laboratories, Albuquerque, NM.

R. L. Iman, J. C. Helton and J. E. Campbell, 1978. Risk Methodology for Geologic Disposal of Radioactive Waste: Sensitivity Analysis Techniques, NUREG/CR-0394, SAND78-0912, Sandia National Laboratories, Albuquerque, NM.

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NUTRAN

Model Type: Systems Model

Author: B. Ross
The Analytic Sciences Corp.
6 Jacob Way
Reading, MA 81867

Sponsoring Agency: USNRC

Availability: Through author

Programming:

(i) Language: PL/1, FORTRAN
(ii) System: IBM 370

Description:

(i) Summary: NUTRAN is a package of computer models capable of calculating the potential dose to humans from a deep geologic repository. The models include ORIGEN, WASTE, BIODOSE and PLOT. The ORIGEN code was developed at Oak Ridge National Laboratory and is used to calculate the inventory of radionuclides in the waste as a function of time. The WASTE program considers a number of ground water related processes including repository resaturation, leaching of the waste matrix, dissolution of leached waste and transport through the ground water system. Transport within the ground water system is modeled as a number of 1-D flow paths (stream tubes). The output of each stream tube is calculated from the input concentration using a Greens Function approach. This output serves as input into subsequent branches. Flux into branching paths is ratioed in accordance with flow rates in the branches.

BIODOSE simulates soil and water bodies as completely mixed compartments. Potential pathways to man which are considered include aquatic food, irrigated crops, animal products, drinking water and ground exposure. Dose resulting from inhalation or

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atmospheric immersion is not considered. Dose commitments are calculated for average and maximum exposed individual as well as total population. Scenario effects can be included as occurring at specified times or according to certain probabilities.

(ii) Inputs:
- inventory description
- stream tube geometry, hydrogeological characteristics, hydraulic heads
- repository geometry
- compartment volumes, transfer coefficients, usage rates, dose factors

(iii) Outputs: 50-year dose commitment to average and maximum exposed individual and total population dose.

Validation: None reported.

Verification: None reported.

Quality Assurance: None reported.

Review Reference: B. I. Ross et al., 1980. User's Guide to NUTRAN: A Computer Analysis System for Long-Term Repository Safety. AECLTR-121.

Documentation: B. I. Ross et al., 1979. NUTRAN: A Computer Model of Long-Term Hazards from Waste Repositores". UCRL-15150, TASC.

B. I. Ross et al., 1980. User's Guide to NUTRAN: A Computer Analysis System for Long-Term Repository Safety. AECL TR-121.

PRESTO

Model Type: Systems Model

Author: C. A. Little, C. J. Emerson, D. E. Fields
and G. Hiromoto
Health and Safety Research Division
Oak Ridge National Laboratory

Sponsoring Agency: USEPA

Programming:

(i) Language: FORTRAN
(ii) System: IBM 360

Description:

(i) Summary: This model is currently undergoing independent modification by both ORNL and EPA. The model described herein is based on an interim version of PRESTO (Prediction of Radiation Effects from Shallow Trench Operations) which includes the basic environmental processes through air, surface and ground water. The final version of the model will address four basic scenarios (1) normal operation with operational spillage, (2) human intrusion, (3) site reclamation by farming, and (4) erosion of facility and subsequent atmospheric suspension. Only the initial operational scenario is fully operational in this (interim) version of PRESTO. PRESTO consists of three types of submodels: (1) unit response models, (2) scheduled event models and (3) risk evaluation models. Processes which are addressed by the model include leaching, trench overflow, cap failure (based on soil erosion), 1-D ground water transport, atmospheric transport resuspension dose to humans based on ingestion, exposure, inhalation and expected health risks. Leach calculations can be based on distribution coefficients or solubilities in conjunction with a fractional or completely mixed assumption based on the amount of water entering the facility over a time step. Infiltration is based on a water balance of run-off precipitation, irrigation and evaporation.

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Surface water contributions are based upon the user-specified fraction of infiltration entering a stream. It would appear ground water contributions to surface water bodies are not considered. Soil erosion is calculated by the Universal Soil Loss equation. Atmospheric suspension may occur through either a user-specified resuspension factor for mechanical resuspension or an empirically-based factor for operational cases. Major assumptions/simplifications contained in this model include (i) daughter products of long decay chains are not considered, (ii) chemical reactions not considered, and (iii) homogeneous waste inventory. Currently this model is set for a 1000-year simulation. Dose calculations and risk assessment calculations are made by DARTAB for ingestion, immersion, exposure and inhalation pathways.

(ii) Inputs: Cap failure as a function of time, trench geometry, hydrogeological parameters, waste density, inventory description and properties, aquifer geometry, ground water velocity, universal soil loss factors, meteorological data, source/receptor distances, mean wind speed, gravitational and deposition velocities, roughness factor, stream flow rates, run-off fraction, fraction of soluble contaminants going to stream, intake rates and times, agricultural productivities, transfer factors.

(iii) Outputs:

- annual dose commitments for specified individual, average individual, collective population dose
- life loss per premature death
- dose by organ or total body

Validation: Not reported.

Verification: Independent submodels may have been verified.

Quality Assurance: Not reported.

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Review Reference: C. A. Little et al., Environmental Assessment Model for Shallow Land Disposal of Low-Level Radioactive Wastes: Interim Report, Oak Ridge National Laboratory, DE81030434, ORNL-5692.

C. L. Bergovich et al., DARTAB: A Program to Combine Airborne Radionuclide Environmental Exposure Data with Dosimetric and Health Effects Data to Generate Tabulations of Predicted Health Impacts, Oak Ridge National Laboratory.

SYVAC

Model Type: Systems Model

Author: K. W. Dormuth and R. D. Quick

Sponsoring Agency: Atomic Energy of Canada Ltd.

Availability: Unknown

Description:

(i) Summary: SYVAC (Systems Variability Analysis Code) comprises three main submodels, one representing each of the vault, geosphere and biosphere regions. The Vault Model is a steady-state model (assuming resaturation and ground water equilibrium have been re-established) considering such processes as container failure, dissolution of the waste matrix and transport through the buffer by advection and/or diffusion. The Geosphere Model addresses the transport of radionuclides in ground water using output from the Vault Model as a source term and generating output for use as input in the Biosphere Model. The Geosphere Model uses a number of simplifying assumptions and reduces the problem to a set of three partial differential equations based on material balances for a three-member decay chain. Major assumptions include: (1) considering advection only, (2) adsorption mechanisms are reversible and (3) steady-state ground water flow system exists. The transport equations included in SYVAC are solved assuming a unit impulse using Laplace transforms. The Biosphere Model assumes that radionuclides reach man through either terrestrial food chains or aquatic food chains. FOODII and NEPTUN are two submodels which are used for these calculations. Processes which require a long time to reach equilibrium are modeled transiently using compartment models and fractional transfer rates (e.g., concentrations in a lake), while a steady-state model is used to compute dose

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to man via his diet. SYVAC is currently oriented towards a Monte Carlo simulation which results in a probability distribution function of the dependent variables based on the assigned probability density distributions of input variables.

(ii) Inputs:
- inventory and properties, vault geometry and properties
- hydrogeological properties
- compartment volumes, transfer coefficients, distribution coefficients
- diet characteristics
- all major iput parameters require probability distribution functions

(iii) Outputs:
- 50 year dose commitments for children and adults

Validation: Various submodels have been validated.

Verification: Various submodels have been verified.

Quality Assurance: Not reported.

Review Reference: D. M. Wuschke et al., 1981. Environmental and Safety Assessment Studies for Nuclear Fuel Waste Management. Volume 3: Post-Closure Assessment. TR-127-3, Whiteshell Nuclear Research Establishment.

Documentation/ Reference : K. W. Dormuth and G. R. Sherman, 1981. SYVAC - A Computer Program for Assessment of Nuclear Fuel Waste Management Systems, Incorporating Parameter Variability. AECL-6814, Whiteshell Nuclear Research Establishment.

D. M. Wuschke et al., 1981. Environmental and Safety Assessment Studies for Nuclear Fuel Waste Management. Volume 3: Post-Closure Assessment. TR-127-3, Whiteshell Nuclear Research Establishment.

R. B. Lyon, 1981. Environmental and Safety Assessment for Nuclear Waste Disposal - The Canadian Approach. Proc. Waste Management '81 Symp. Tucson, Arizona.